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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS 3	JUN 06	KOREAPAT updated with 41,000 documents
NEWS 4	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS 5	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS 6	JUN 25	CA/CAplus and USPAT databases updated with IPC reclassification data
NEWS 7	JUN 30	AEROSPACE enhanced with more than 1 million U.S. patent records
NEWS 8	JUN 30	EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations
NEWS 9	JUN 30	STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in
NEWS 10	JUN 30	STN AnaVist enhanced with database content from EPFULL
NEWS 11	JUL 28	CA/CAplus patent coverage enhanced
NEWS 12	JUL 28	EPFULL enhanced with additional legal status information from the epoline Register
NEWS 13	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS 14	JUL 28	STN Viewer performance improved
NEWS 15	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS 16	AUG 13	CA/CAplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS 17	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS 18	AUG 15	CAplus currency for Korean patents enhanced
NEWS 19	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS 20	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued
NEWS 21	SEP 25	CA/CAplus current-awareness alert options enhanced to accommodate supplemental CAS indexing of exemplified prophetic substances
NEWS 22	SEP 26	WPIDS, WPINDEX, and WPIX coverage of Chinese and and Korean patents enhanced
NEWS 23	SEP 29	IFICLS enhanced with new super search field
NEWS 24	SEP 29	EMBASE and EMBAL enhanced with new search and display fields
NEWS 25	SEP 30	CAS patent coverage enhanced to include exemplified prophetic substances identified in new Japanese-language patents
NEWS 26	OCT 07	EPFULL enhanced with full implementation of EPC2000
NEWS 27	OCT 07	Multiple databases enhanced for more flexible patent number searching

```
 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:03:15 ON 20 OCT 2008

=> fil reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.42       0.42

FILE 'REGISTRY' ENTERED AT 08:04:28 ON 20 OCT 2008
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STRUCTURE FILE UPDATES:   17 OCT 2008  HIGHEST RN 1062752-24-2
DICTIONARY FILE UPDATES:  17 OCT 2008  HIGHEST RN 1062752-24-2

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TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

  Please note that search-term pricing does apply when
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REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\QUERIES\105384521.str
```

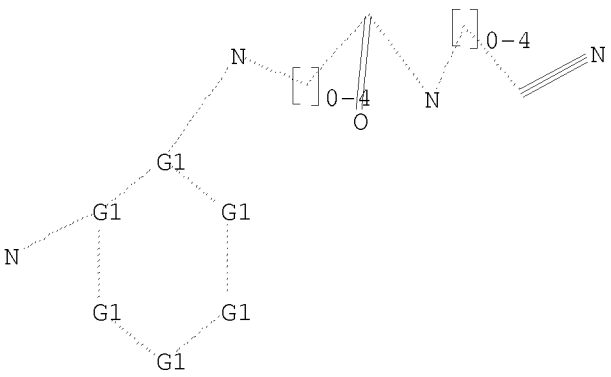
chain nodes :
10 11 12 13 14 15 16 17
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
9
chain bonds :
3-9 6-10 10-11 11-12 12-13 12-17 13-14 14-15 15-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 3-9 4-5 5-6 6-10 10-11 11-12 12-13 12-17 13-14 14-15
15-16

G1:C,N

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 9:CLASS 10:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

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=> s l1
SAMPLE SEARCH INITIATED 08:04:50 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     5038 TO ITERATE

 39.7% PROCESSED     2000 ITERATIONS                                 1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         96504 TO   105016
PROJECTED ANSWERS:                1 TO      145

L2             1 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 08:04:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   101953 TO ITERATE

100.0% PROCESSED   101953 ITERATIONS                               11 ANSWERS
SEARCH TIME: 00.00.02

L3            11 SEA SSS FUL L1

=> s l3 and caplus/lc
      59346897 CAPLUS/LC
L4            1 L3 AND CAPLUS/LC

=> s l3 not l4
L5           10 L3 NOT L4

=> d l5 1-10
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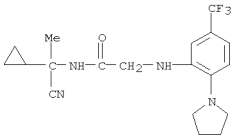
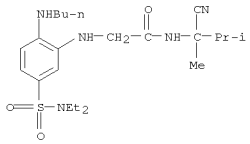
L5 ANSWER 1 OF 10 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1043119-89-6 REGISTRY
ED Entered STN: 24 Aug 2008
CN Acetamide, N-(1-cyano-1-cyclopropylethyl)-2-[[2-(1-pyrrolidinyl)-5-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)
MF C19 H23 F3 N4 O
SR Chemical Library
Supplier: UkrOrgSynthesis
LC STN Files: CHEMCATS



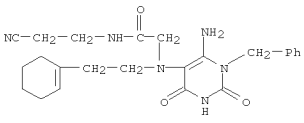
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 2 OF 10 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1015321-16-0 REGISTRY
ED Entered STN: 17 Apr 2008
CN Acetamide, 2-[[2-(butylamino)-5-[(diethylamino)sulfonyl]phenyl]amino]-N-(1-cyano-1,2-dimethylpropyl)- (CA INDEX NAME)
MF C22 H37 N5 O3 S
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



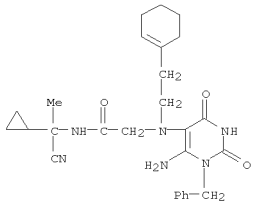
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 3 OF 10 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1011230-38-8 REGISTRY
ED Entered STN: 01 Apr 2008
CN Acetamide, 2-[[6-amino-1,2,3,4-tetrahydro-2,4-dioxo-1-(phenylmethyl)-5-pyrimidinyl][2-(1-cyclohexen-1-yl)ethyl]amino]-N-(2-cyanoethyl)- (CA INDEX NAME)
MF C24 H30 N6 O3
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



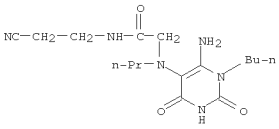
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 4 OF 10 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1011230-26-4 REGISTRY
ED Entered STN: 01 Apr 2008
CN Acetamide, 2-[[6-amino-1,2,3,4-tetrahydro-2,4-dioxo-1-(phenylmethyl)-5-pyrimidinyl][2-(1-cyclohexen-1-yl)ethyl]amino]-N-(1-cyano-1-cyclopropylethyl)- (CA INDEX NAME)
MF C27 H34 N6 O3
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



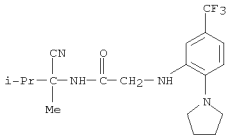
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 5 OF 10 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1011223-40-7 REGISTRY
ED Entered STN: 01 Apr 2008
CN Acetamide, 2-[(6-amino-1-butyl-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)propylamino]-N-(2-cyanoethyl)- (CA INDEX NAME)
MF C16 H26 N6 O3
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



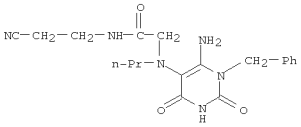
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 6 OF 10 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1011162-92-7 REGISTRY
ED Entered STN: 31 Mar 2008
CN Acetamide, N-(1-cyano-1,2-dimethylpropyl)-2-[[2-(1-pyrrolidinyl)-5-(trifluoromethyl)phenyl]amino]- (CA INDEX NAME)
MF C19 H25 F3 N4 O
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



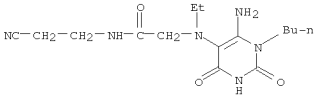
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 7 OF 10 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1011112-14-3 REGISTRY
ED Entered STN: 31 Mar 2008
CN Acetamide, 2-[[6-amino-1,2,3,4-tetrahydro-2,4-dioxo-1-(phenylmethyl)-5-pyrimidinyl]propylamino]-N-(2-cyanoethyl)- (CA INDEX NAME)
MF C19 H24 N6 O3
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



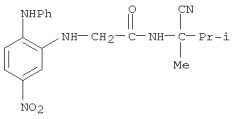
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 8 OF 10 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1010681-26-1 REGISTRY
ED Entered STN: 28 Mar 2008
CN Acetamide, 2-[(6-amino-1-butyl-1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)ethylamino]-N-(2-cyanoethyl)- (CA INDEX NAME)
MF C15 H24 N6 O3
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



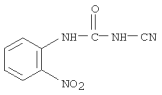
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 9 OF 10 REGISTRY COPYRIGHT 2008 ACS on STN
RN 924061-34-7 REGISTRY
ED Entered STN: 01 Mar 2007
CN Acetamide, N-(1-cyano-1,2-dimethylpropyl)-2-[[5-nitro-2-(phenylamino)phenyl]amino]- (CA INDEX NAME)
MF C20 H23 N5 O3
SR Chemical Library
Supplier: Aurora Fine Chemicals
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 10 OF 10 REGISTRY COPYRIGHT 2008 ACS on STN
RN 500294-33-7 REGISTRY
ED Entered STN: 24 Mar 2003
CN Urea, N-cyano-N'-(2-nitrophenyl)- (CA INDEX NAME)
OTHER NAMES:
CN NSC 86942
MF C8 H6 N4 O3
SR Chemical Library



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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=> fil caplus
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     204.89     205.31

FILE 'CAPLUS' ENTERED AT 08:06:43 ON 20 OCT 2008
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FILE COVERS 1907 - 20 Oct 2008  VOL 149 ISS 17
FILE LAST UPDATED: 19 Oct 2008  (20081019/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> d his

     (FILE 'HOME' ENTERED AT 08:03:15 ON 20 OCT 2008)

     FILE 'REGISTRY' ENTERED AT 08:04:28 ON 20 OCT 2008
L1             STRUCTURE UPLOADED
L2           1 S L1
L3          11 S L1 FULL
L4           1 S L3 AND CAPLUS/LC
L5          10 S L3 NOT L4

     FILE 'CAPLUS' ENTERED AT 08:06:43 ON 20 OCT 2008

=> s l4
L6           2 L4

=> d ibib abs hitstr 1-2
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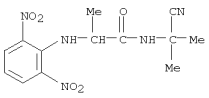
L6 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:437778 CAPLUS
DOCUMENT NUMBER: 71:37778
ORIGINAL REFERENCE NO.: 71:6953a,6956a
TITLE: Selection of a candidate herbicide; a study of structure-activity effects in a series of amino acid derivatives
AUTHOR(S): Yates, J.
CORPORATE SOURCE: Woodstock Agr. Res. Centre, Sittingbourne, UK
SOURCE: Proc. Brit. Weed Contr. Conf., 9th (1968), Volume 2, 659-67. Brit. Crop Prot. Counc.: Droitwich, Engl. CODEN: 20YZAP
DOCUMENT TYPE: Conference
LANGUAGE: English

AB A group of herbicidal compds. have been developed from N-(phenyl)alanine, a known growth-regulating chemical Highly specific requirements for activity were encountered in the series ArNHRCOY in which H2NRCO2H represents an amino acid. Maximum effect was observed in the D-form of 2-(4-methyl-2,6-dinitroanilino)-N-methylpropionamide. The active herbicides were more toxic to seeds than to seedling plants, in which they induced scorch and chlorosis. They did not act as uncouplers of oxidative phosphorylation or inhibit the Hill reaction. The mode of activity is unclear, but they may interfere with peptide synthesis.

IT 19383-24-5
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(herbicidal activity of)
RN 19383-24-5 CAPLUS
CN Propionamide, N-(1-cyano-1-methylethyl)-2-(2,6-dinitroanilino)- (8CI) (CA INDEX NAME)



L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1968:467079 CAPLUS
DOCUMENT NUMBER: 69:67079
ORIGINAL REFERENCE NO.: 69:12515a,12518a
TITLE: Herbicidal anilinoalkanamides
PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij N. V.
SOURCE: Neth. Appl., 41 pp.
CODEN: NAXXAN
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6707890		19671211	NL 1967-7890	19670607
DE 1642337			DE	
FR 1525715			FR	
GB 1122043			GB	
US 3634509		19720111	US	19690903
US 3734711		19730522	US	19710315
PRIORITY APPLN. INFO.:			GB	19660608
			GB	19670502

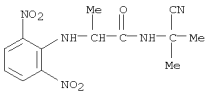
GI For diagram(s), see printed CA Issue.

AB The title compds. of the general formula I, where the symbols have the tabulated values, were prepared either by treating the corresponding chlorobenzene with the corresponding amino acid in EtOH in the presence of NaHCO3 at 70-120°, refluxing the formed acid in C6H6 with thionyl chloride (II), and treating the formed acid chloride with the corresponding amine in CH2Cl2 at a temperature between -20° and +30°, or by treating the corresponding aniline with the corresponding BrCHR(CH2)nCO2Et at 80-120°, and treating the formed ester with the corresponding amine in EtOH at 100-50°. Thus, a mixture of 1-chloro-2,6-dinitrobenzene 810, DL-alanine 384, and NaHCO3 840 g. was stirred and refluxed 18 hrs. in 8 l. 95% EtOH and the mixture diluted with 4 l. water, filtered, distilled in vacuo while adding 4 l. water to remove EtOH, cooled by adding 2 l. ice, acidified with concentrated HCl, and stirred to give 95% 2-(2,6-dinitroanilino)propionic acid (III), m. 137-8°. To a solution of 490 g. III in 2.5 l. C6H6 570 g. II was added while stirring and the mixture stirred and refluxed 12 hrs., filtered, and distilled to remove C6H6 and excess II. To a solution of the residual oil in 2.5 l. CH2Cl2, a solution of 160 g. NH2Me in 1 l. Ch2Cl2 was added while stirring at 0-5°, the mixture filtered, the filtrate evaporated, and the residue stirred with 1 l. tech. denaturated alc. to give 61% I (X2 = X6 = NO2, X3 = X4 = X5 = H, R = Me; n = 0, R1 = H, R2 = Me) m. 146-8°. Similarly prepared I are given in Table 1, page 6259. A mixture of 2,5-dichloroani line 324 and ethyl 2-bromopropionate 18.1 g. was heated 5 hrs. at 100°, water added to the hot melt, the organic phase extracted with Et2O, the extract evaporated, and the residue fractionally distilled in vacuo to give 7 g. ethyl 2-(2,5-dichloroanilino)propionate (IV), b0.9

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

127-30°. IV (10 g.) was heated 15 hrs. at 120° with 50 cc. 33 wt./vol. % soln. of NH2Me in EtOH in a closed tube and the reaction mixt. was concd., filtered hot, and allowed to cool to give 70% I (X2 = X5 = Cl, X3 = X4 = X6 = H, R = Me, n = 0, R1 = H, R2 = Me), m. 168-9° (EtOH). Similarly prepd. I are given in Table 2.

IT 19383-24-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 19383-24-5 CAPLUS
CN Propionamide, N-(1-cyano-1-methylethyl)-2-(2,6-dinitroanilino)- (8CI) (CA INDEX NAME)



=> fil reg
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 11.38 | 216.69

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION
CA SUBSCRIBER PRICE | -1.60 | -1.60

FILE 'REGISTRY' ENTERED AT 08:07:23 ON 20 OCT 2008

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

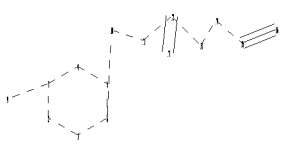
STRUCTURE FILE UPDATES: 17 OCT 2008 HIGHEST RN 1062752-24-2
DICTIONARY FILE UPDATES: 17 OCT 2008 HIGHEST RN 1062752-24-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

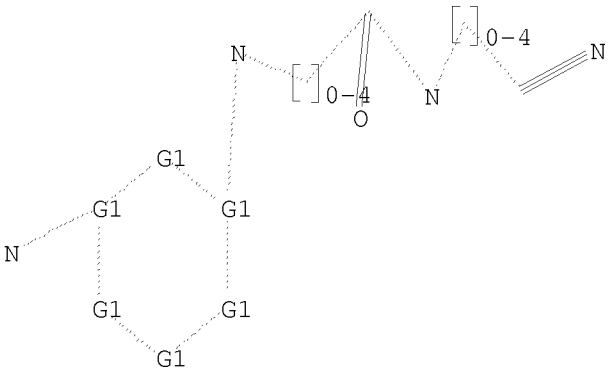
TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of



L7 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

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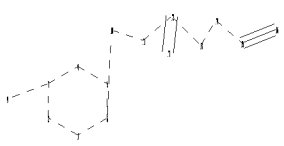
SAMPLE SCREEN SEARCH COMPLETED - 5038 TO ITERATE

39.7% PROCESSED 2000 ITERATIONS 2 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01



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FULL SUBSET SCREEN SEARCH COMPLETED -       30 TO ITERATE

100.0% PROCESSED       30 ITERATIONS                             30 ANSWERS
SEARCH TIME: 00.00.01

L11          30 SEA SUB=L9 SSS FUL L10

=> s l9 not l12
L12 NOT FOUND
The L-number entered could not be found.  To see the definition
of L-numbers, enter DISPLAY HISTORY at an arrow prompt (=>).

=> s l9 not l11
L12         46 L9 NOT L11

=> s l12 and caplus/lc
      59346897 CAPLUS/LC
L13         37 L12 AND CAPLUS/LC

=>  s l12 not l13
L14          9 L12 NOT L13

=> d l14 1-9
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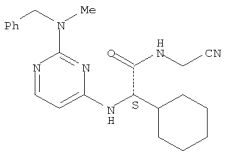
L14 ANSWER 1 OF 9 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1028318-12-8 REGISTRY
ED Entered STN: 15 Jun 2008
CN INDEX NAME NOT YET ASSIGNED
FS STEREOSEARCH
MF C22 H28 N6 O
SR Other Sources
Database: ChemSpider (ChemZoo, Inc.)

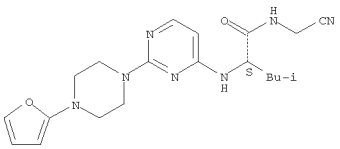
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 ANSWER 2 OF 9 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1027994-97-3 REGISTRY
ED Entered STN: 13 Jun 2008
CN Pentanamide, N-(cyanomethyl)-2-[[2-[4-(2-furanyl)-1-piperazinyl]-4-pyrimidinyl]amino]-4-methyl-, (2S)- (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H27 N7 O2
SR Other Sources
Database: ChemSpider (ChemZoo, Inc.)

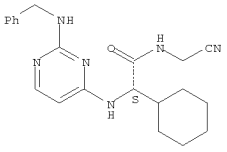
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 ANSWER 3 OF 9 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1026334-50-8 REGISTRY
ED Entered STN: 08 Jun 2008
CN Cyclohexaneacetamide, N-(cyanomethyl)-α-[[2-[(phenylmethyl)amino]-4-pyrimidinyl]amino]-, (αS)- (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H26 N6 O
SR Other Sources
Database: ChemSpider (ChemZoo, Inc.)

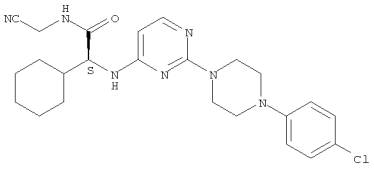
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 ANSWER 4 OF 9 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1025986-08-6 REGISTRY
ED Entered STN: 06 Jun 2008
CN Cyclohexaneacetamide, α-[[2-[4-(4-chlorophenyl)-1-piperazinyl]-4-pyrimidinyl]amino]-N-(cyanomethyl)-, (αS)- (CA INDEX NAME)
FS STEREOSEARCH
MF C24 H30 Cl N7 O
SR Other Sources
Database: ChemSpider (ChemZoo, Inc.)

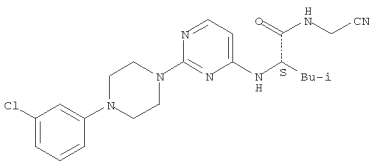
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 ANSWER 5 OF 9 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1025973-30-1 REGISTRY
ED Entered STN: 06 Jun 2008
CN Pentanamide,
2-[[2-[4-(3-chlorophenyl)-1-piperazinyl]-4-pyrimidinyl]amino]-
N-(cyanomethyl)-4-methyl-, (2S)- (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H28 Cl N7 O
SR Other Sources
Database: ChemSpider (ChemZoo, Inc.)

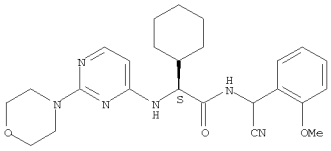
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 ANSWER 6 OF 9 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1025804-87-8 REGISTRY
ED Entered STN: 05 Jun 2008
CN Cyclohexaneacetamide, N-[cyano(2-methoxyphenyl)methyl]-α-[[2-(4-
morpholinyl)-4-pyrimidinyl]amino]-, (αS)- (CA INDEX NAME)
FS STEREOSEARCH
MF C25 H32 N6 O3
SR Other Sources
Database: ChemSpider (ChemZoo, Inc.)

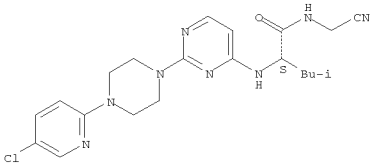
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 ANSWER 7 OF 9 REGISTRY COPYRIGHT 2008 ACS on STN
RN 714216-35-0 REGISTRY
ED Entered STN: 22 Jul 2004
CN Pentanamide, 2-[[2-[4-(5-chloro-2-pyridinyl)-1-piperazinyl]-4-
pyrimidinyl]amino]-N-(cyanomethyl)-4-methyl-, (2S)- (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H27 Cl N8 O
CI COM
SR CA

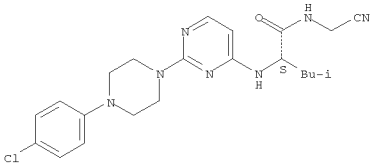
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 ANSWER 8 OF 9 REGISTRY COPYRIGHT 2008 ACS on STN
RN 714216-33-8 REGISTRY
ED Entered STN: 22 Jul 2004
CN Pentanamide,
2-[[2-[4-(4-chlorophenyl)-1-piperazinyl]-4-pyrimidinyl]amino]-
N-(cyanomethyl)-4-methyl-, (2S)- (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H28 Cl N7 O
CI COM
SR CA

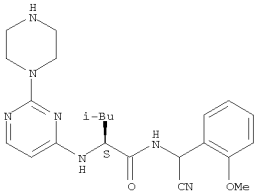
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L14 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2008 ACS on STN
RN   714216-18-9 REGISTRY
ED   Entered STN: 22 Jul 2004
CN   Pentanamide, N-[cyano(2-methoxyphenyl)methyl]-4-methyl-2-[[2-(1-piperazinyl)-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)
FS   STEREOSEARCH
MF   C23 H31 N7 O2
CI   COM
SR   CA

Absolute stereochemistry.



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FULL ESTIMATED COST                                        244.99     461.68

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)              SINCE FILE      TOTAL
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FILE COVERS 1907 - 20 Oct 2008  VOL 149 ISS 17
FILE LAST UPDATED: 19 Oct 2008  (20081019/ED)

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reclassification data for the second quarter of 2008.

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L3          11 S L1 FULL
L4           1 S L3 AND CAPLUS/LC
L5          10 S L3 NOT L4

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L6           2 S L4

     FILE 'REGISTRY' ENTERED AT 08:07:23 ON 20 OCT 2008
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L8           2 S L7
L9          76 S L7 FULL
L10            STRUCTURE UPLOADED
L11         30 S L10 FULL SUB=L9
L12         46 S L9 NOT L11
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L13           37 S L12 AND CAPLUS/LC
L14            9 S L12 NOT L13

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=> s l13
L15           4 L13

=> d ibib abs hitstr 1-4
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L15 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

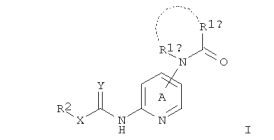
ACCESSION NUMBER: 2008:473550 CAPLUS
DOCUMENT NUMBER: 148:449469
TITLE: Preparation of 2-aminopyridine derivatives as glycogen synthase 3 (GSK-3β) inhibitors
INVENTOR(S): Kori, Masakuni; Oki, Hideyuki; Tsukamoto, Tetsuya; Takahashi, Masashi; Setoh, Masaki; Hirano, Takehiro
PATENT ASSIGNEE(S): Takeda Pharmaceutical Company Limited, Japan
SOURCE: PCT Int. Appl., 179pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008044700	A1	20080417	WO 2007-JP69738	20071010
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

PRIORITY APPLN. INFO.: JP 2006-278026 A 20061011

OTHER SOURCE(S): MARPAT 148:449469
GI

L15 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



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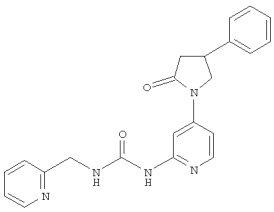


II

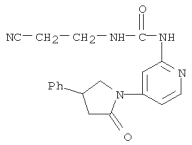
AB The title compds. including N-(2-pyridyl)urea, -benzamides, and -alkanamides [I; R1a = H, each (un)substituted hydrocarbyl or heterocyclyl; R1b = each (un)substituted hydrocarbyl, hydrocarbyloxy, or monocyclic heterocyclyl; or R1aNCORb together represents (un)substituted oxo-mono or tricyclic N-containing heterocyclyl; R2 = each (un)substituted hydrocarbyl or heterocyclyl; X = (un)substituted NH, O, CONH, bond; Y = O, S; ring A = pyridine ring optionally substituted by 1-3 substituents selected from halo and lower alkyl] or salts thereof were prepared These compds. are GSK-3β inhibitors and also promoters for differentiation of neural stem cells and are useful as prophylactic/therapeutic agents for a GSK-3β-related condition or disease such as neurodegenerative disease and diabetes. Thus, 0.5 mL 2,2,2-trichloroethyl chloroformate was added to a solution of 532 mg 1-(2-aminopyridin-4-yl)-4-phenylpyrrolidin-2-one and 0.26 mL Et3N in 20 mL THF at 0° and the resulting mixture was stirred for 10 min to give, after workup, an intermediate. The intermediate obtained was stirred with a solution of 0.30 mL 1-(pyridin-2-yl)methanamine, and 0.63 mL diisopropylethylamine in 3 mL DMSO at 70° for 3 h to give, after workup and silica gel chromatog., 30% N-(4-(2-oxo-4-phenylpyrrolidin-1-yl)pyridin-2-yl)-N'-((pyridin-2-yl)methyl)urea (II). II in vitro showed IC50 of <100 nM against recombinant human GSK-3β. Pharmaceutical formulations, e.g. a tablet containing N-Benzyl-N'-(4-(2-oxopyrrolidin-1-yl)pyridin-2-yl)urea, were described.

IT 1019648-64-6P, N-(2-Cyanoethyl)-N'-[4-(2-oxo-4-phenylpyrrolidin-1-yl]urea

L15 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 2-aminopyridine derivs. as glycogen synthase 3 (GSK-3β) inhibitors and promoters for differentiation of neural stem cell for prevention and/or treatment of neurodegenerative disease and diabetes)

RN 1019648-64-6 CAPLUS
CN Urea,
N-(2-cyanoethyl)-N'-[4-(2-oxo-4-phenyl-1-pyrrolidinyl)-2-pyridinyl]- (CA INDEX NAME)



REFERENCE COUNT: 81 THERE ARE 81 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:534183 CAPLUS
DOCUMENT NUMBER: 141:89367
TITLE: Preparation of amino acid derivatives as cathepsin cysteine protease inhibitors
INVENTOR(S): Mcinally, Judith; Pairaudeau, Garry; Patel, Anil; Thom, Stephen
PATENT ASSIGNEE(S): Astrazeneca Ab, Swed.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004054987	A1	20040701	WO 2003-SE1931	20031211
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003303076	A1	20040709	AU 2003-303076	20031211
EP 1572667	A1	20050914	EP 2003-813325	20031211
EP 1572667	B1	20070509		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006514948	T	20060518	JP 2004-560214	20031211
AT 361914	T	20070615	AT 2003-813325	20031211
ES 2285273	T3	20071116	ES 2003-813325	20031211
US 20060111364	A1	20060525	US 2005-538452	20050610
PRIORITY APPLN. INFO.:			SE 2002-3712 A	20021213
			WO 2003-SE1931 W	20031211

OTHER SOURCE(S): MARPAT 141:89367

AB The invention relates to compds. R1R2N-Het-NR3CR4R5CONR6CR7R8CN [R1 is H, alkyl or cycloalkyl; R2 is aryl, heteroaryl, alkyl-R9, CO(alkyl)R9 or SO2(alkyl)R9, where R9 is aryl or heteroaryl; or R1R2N is a 4 to 7-membered saturated ring optionally containing a carbonyl group, O, S or N atom and optionally substituted; Het is a (un)substituted heteroaryl ring chosen from pyridine, pyrimidine, pyrazine, pyridazine or triazine; R3, R5, R6, R7 are H, alkyl or cycloalkyl; R4 is H, (un)substituted alkyl, cycloalkyl, arylalkyl or heteroarylalkyl; R8 is H, aryl, heteroaryl of (un)substituted alkyl] or their pharmaceutically-acceptable salts for use in treating diseases associated with cysteine protease activity, particular cathepsin S. Thus, N-(2-morpholino-4-pyrimidinyl)-L-leucine cyano(2-methoxyphenyl)methylamide was prepared by amidation of Boc-L-Leu-OH (Boc = tert-butoxycarbonyl) with 2-MeOC6H4CH(NH2)CN, followed by deprotection with formic acid and reaction with 2,4-difluoropyrimidine and

morpholine.

IT 714216-17-8P 714216-19-0P 714216-20-3P
714216-21-4P 714216-22-5P 714216-23-6P
714216-24-7P 714216-25-8P 714216-26-9P
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714216-30-5P 714216-31-6P 714216-32-7P
714216-34-9P 714216-36-1P 714216-37-2P
714216-38-3P 714216-39-4P 714216-40-7P
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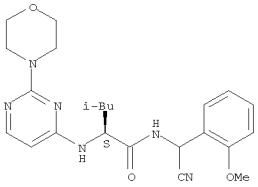
714216-50-9P 714216-51-0P 714216-52-1P
714216-53-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid derivs. as cathepsin cysteine protease inhibitors)

RN 714216-17-8 CAPLUS
CN Pentanamide, N-[cyano(2-methoxyphenyl)methyl]-4-methyl-2-[[2-(4-morpholinyl)-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

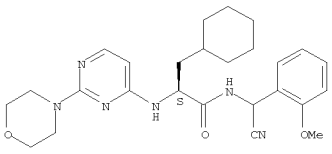


RN 714216-19-0 CAPLUS
CN Pentanamide, N-[cyano(2-methoxyphenyl)methyl]-4-methyl-2-[[2-(1-piperazinyl)-4-pyrimidinyl]amino]-, (2S)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

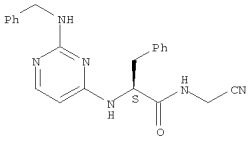
CRN 714216-18-9
CMF C23 H31 N7 O2

Absolute stereochemistry.



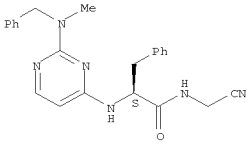
RN 714216-22-5 CAPLUS
CN Benzenepropanamide, N-(cyanomethyl)-α-[[2-[(phenylmethyl)amino]-4-pyrimidinyl]amino]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



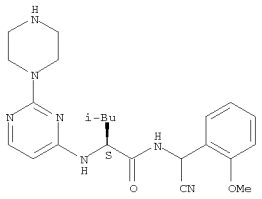
RN 714216-23-6 CAPLUS
CN Benzenepropanamide, N-(cyanomethyl)-α-[[2-[methyl(phenylmethyl)amino]-4-pyrimidinyl]amino]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



RN 714216-24-7 CAPLUS
CN Benzenepropanamide, α-[[2-[4-(4-chlorophenyl)-1-piperazinyl]-4-pyrimidinyl]amino]-N-(cyanomethyl)-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.

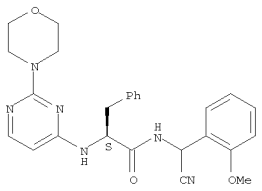


CM 2

CRN 76-05-1
CMF C2 H F3 O2

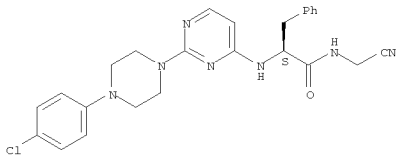
RN 714216-20-3 CAPLUS
CN Benzenepropanamide, N-[cyano(2-methoxyphenyl)methyl]-α-[[2-(4-morpholinyl)-4-pyrimidinyl]amino]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



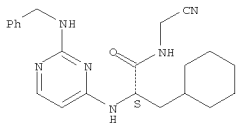
RN 714216-21-4 CAPLUS
CN Cyclohexanepropanamide, N-[cyano(2-methoxyphenyl)methyl]-α-[[2-(4-morpholinyl)-4-pyrimidinyl]amino]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



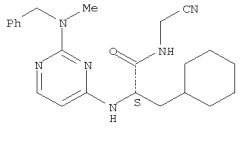
RN 714216-25-8 CAPLUS
CN Cyclohexanepropanamide, N-(cyanomethyl)-α-[[2-[(phenylmethyl)amino]-4-pyrimidinyl]amino]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



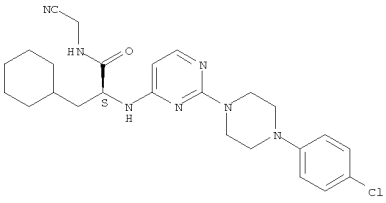
RN 714216-26-9 CAPLUS
CN Cyclohexanepropanamide, N-(cyanomethyl)-α-[[2-[methyl(phenylmethyl)amino]-4-pyrimidinyl]amino]-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



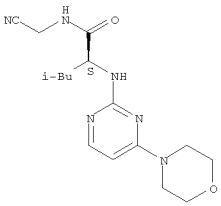
RN 714216-27-0 CAPLUS
CN Cyclohexanepropanamide, α-[[2-[4-(4-chlorophenyl)-1-piperazinyl]-4-pyrimidinyl]amino]-N-(cyanomethyl)-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.



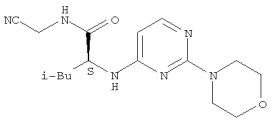
RN 714216-28-1 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[4-(4-morpholinyl)-2-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



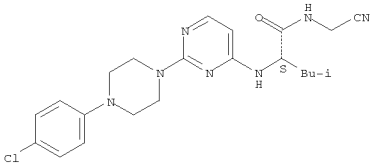
RN 714216-29-2 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[2-(4-morpholinyl)-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 714216-30-5 CAPLUS
CN Pentanamide, N-(cyanomethyl)-2-[[2-(4-hydroxy-4-phenyl-1-piperidinyl)-4-pyrimidinyl]amino]-4-methyl-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



CM 2

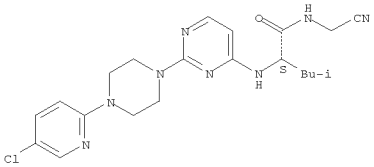
CRN 76-05-1
CMF C2 H F3 O2

RN 714216-36-1 CAPLUS
CN Pentanamide, 2-[[2-[4-(5-chloro-2-pyridinyl)-1-piperazinyl]-4-pyrimidinyl]amino]-N-(cyanomethyl)-4-methyl-, (2S)-, 2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

CM 1

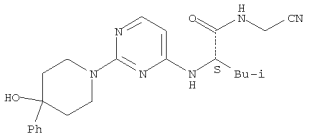
CRN 714216-35-0
CMF C21 H27 Cl N8 O

Absolute stereochemistry.



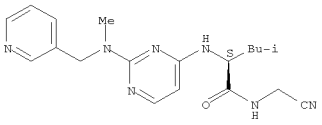
CM 2

Absolute stereochemistry.



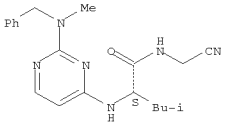
RN 714216-31-6 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[2-[methyl(3-pyridinylmethyl)amino]-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 714216-32-7 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[2-[methyl(phenylmethyl)amino]-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 714216-34-9 CAPLUS
CN Pentanamide, 2-[[2-[4-(4-chlorophenyl)-1-piperazinyl]-4-pyrimidinyl]amino]-N-(cyanomethyl)-4-methyl-, (2S)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

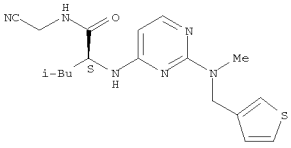
CM 1

CRN 714216-33-8
CMF C22 H28 Cl N7 O

CRN 76-05-1
CMF C2 H F3 O2

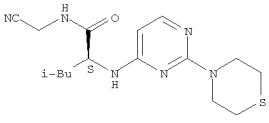
RN 714216-37-2 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[2-[methyl(3-thienylmethyl)amino]-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



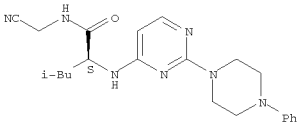
RN 714216-38-3 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[2-(4-thiomorpholinyl)-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



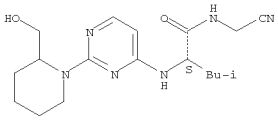
RN 714216-39-4 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[2-(4-phenyl-1-piperazinyl)-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



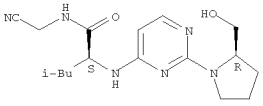
RN 714216-40-7 CAPLUS
CN Pentanamide, N-(cyanomethyl)-2-[[2-[2-(hydroxymethyl)-1-piperidinyl]-4-pyrimidinyl]amino]-4-methyl-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



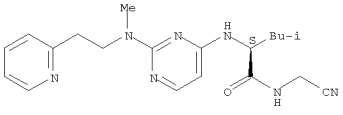
RN 714216-41-8 CAPLUS
CN Pentanamide, N-(cyanomethyl)-2-[[2-[(2R)-2-(hydroxymethyl)-1-pyrrolidinyl]-4-pyrimidinyl]amino]-4-methyl-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



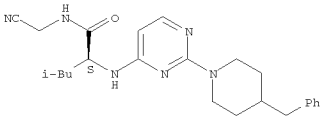
RN 714216-42-9 CAPLUS
CN Pentanamide, N-(cyanomethyl)-2-[[2-(4-hydroxy-1-piperidinyl)-4-pyrimidinyl]amino]-4-methyl-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



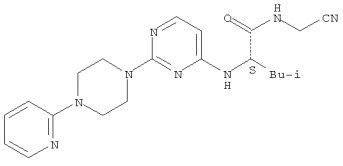
RN 714216-46-3 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[2-[4-(phenylmethyl)-1-piperidinyl]-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



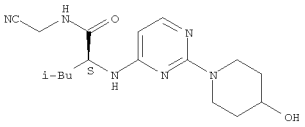
RN 714216-47-4 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[2-[4-(2-pyridinyl)-1-piperazinyl]-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



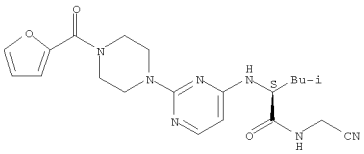
RN 714216-48-5 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[2-(4-phenyl-1-piperidinyl)-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



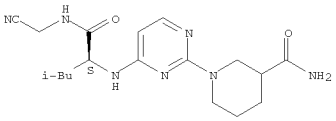
RN 714216-43-0 CAPLUS
CN Pentanamide, N-(cyanomethyl)-2-[[2-[4-(2-furanylcarbonyl)-1-piperazinyl]-4-pyrimidinyl]amino]-4-methyl-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



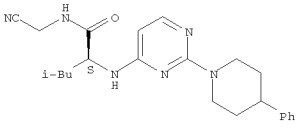
RN 714216-44-1 CAPLUS
CN 3-Piperidinecarboxamide, 1-[4-[[(1S)-1-[[(cyanomethyl)amino]carbonyl]-3-methylbutyl]amino]-2-pyrimidinyl]- (CA INDEX NAME)

Absolute stereochemistry.



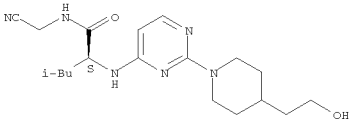
RN 714216-45-2 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[2-[methyl[2-(2-pyridinyl)ethyl]amino]-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



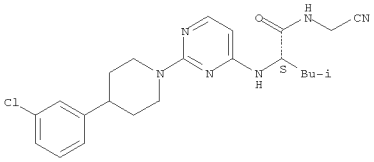
RN 714216-49-6 CAPLUS
CN Pentanamide, N-(cyanomethyl)-2-[[2-[4-(2-hydroxyethyl)-1-piperidinyl]-4-pyrimidinyl]amino]-4-methyl-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 714216-50-9 CAPLUS
CN Pentanamide, 2-[[2-[4-(3-chlorophenyl)-1-piperidinyl]-4-pyrimidinyl]amino]-N-(cyanomethyl)-4-methyl-, (2S)- (CA INDEX NAME)

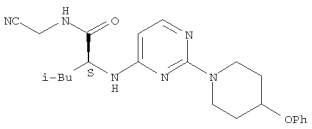
Absolute stereochemistry.



RN 714216-51-0 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[2-(4-phenoxy-1-piperidinyl)-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

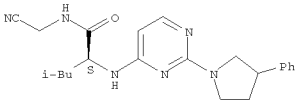
Absolute stereochemistry.

L15 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



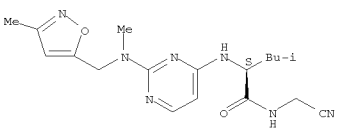
RN 714216-52-1 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[2-(3-phenyl-1-pyrrolidinyl)-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 714216-53-2 CAPLUS
CN Pentanamide, N-(cyanomethyl)-4-methyl-2-[[2-[methyl[(3-methyl-5-isoxazolyl)methyl]amino]-4-pyrimidinyl]amino]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

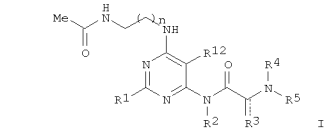
ACCESSION NUMBER: 2003:511098 CAPLUS
DOCUMENT NUMBER: 139:85366
TITLE: Preparation of N-(pyrimidin-4-yl)acetamides as A2b adenosine receptor selective antagonists
INVENTOR(S): Castelhano, Arlindo; McKibben, Bryan; Steinig, Arno; Collington, Eric William
PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 150 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053366	A2	20030703	WO 2002-US41273	20021220
WO 2003053366	A3	20040129		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2471059	A1	20030703	CA 2002-2471059	20021220
AU 2002366811	A1	20030709	AU 2002-366811	20021220
US 20030162764	A1	20030828	US 2002-326204	20021220
US 6916804	B2	20050712		
BR 2002015202	A	20041013	BR 2002-15202	20021220
EP 1465631	A2	20041013	EP 2002-805676	20021220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CN 1620294	A	20050525	CN 2002-828270	20021220
JP 2005517659	T	20050616	JP 2003-554126	20021220
MX 2004PA05862	A	20041101	MX 2004-PA5862	20040616
IN 2004DN01871	A	20070406	IN 2004-DN1871	20040630
US 20050119271	A1	20050602	US 2004-992239	20041118

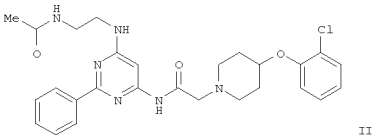
PRIORITY APPLN. INFO.: US 2001-342595P P 20011220
US 2002-326204 A1 20021220
WO 2002-US41273 W 20021220

OTHER SOURCE(S): MARPAT 139:85366
GI

L15 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



I



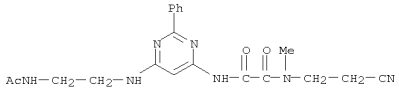
II

AB Title compds. I [wherein R1 = (un)substituted Ph, heterocyclyl, or heteroaryl; R2 and R3 = independently H or (un)substituted (cyclo)alkyl, alkanoyl, alkoxy(carbonyl), alkenyl, monocyclic or bicyclic aryl, heteroaryl, or heterocyclyl; or R2 and R3 are joined to form a heterocyclic ring; wherein the dashed line = a double bond which may be present or absent, and when present R3 = O; R4 and R5 = independently (un)substituted (cyclo)alkyl, alkanoyl, alkoxy(carbonyl), alkenyl, monocyclic or bicyclic aryl, heteroaryl, or heterocyclyl; or NR4R5 = (un)substituted monocyclic or bicyclyl, heterocyclyl, or heteroaryl; R12 = H, alkyl, halo, or cyano; n = 0-4; or enantiomers, tautomers, or pharmaceutically acceptable salts thereof] were prepared as A2b adenosine receptor antagonists. For example, cycloaddn. of benzamidine•HCl and di-Et malonate using DBU in DMF gave 2-phenylpyrimidine-4,6-diol (73%). Chlorination (95%), amination (93%), substitution with N-(2-aminoethyl)acetamide (57%), and amidation with chloroacetyl chloride (91%) provided N-[6-(2-acetylaminoethylamino)-2-phenylpyrimidin-4-yl]-2-chloroacetamide. Coupling of the chloroacetamide with 4-(2-chlorophenoxy)piperidine in the presence of NaI and DIPEA in 3:1 acetonitrile:THF afforded II (86%). Compds. of the invention showed greater than tenfold selectivity for the human A2b adenosine receptor (Ki values <100 nM) over the A1, A2a, and A3 receptors in radioligand binding assays. Thus, I and pharmaceutical comps. comprising I are useful for the treatment of diseases associated with the A2b adenosine receptor, such as asthma, diabetes, or proliferating tumors associated with mast cell degranulation (no data).

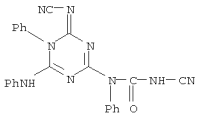
IT 552870-45-8P, N-[6-[[2-(Acetylamino)ethyl]amino]-2-phenylpyrimidin-4-yl]-N'-(2-cyanoethyl)-N'-methylethanediamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(A2b antagonist; preparation of N-(pyrimidinyl)acetamides as A2b adenosine

L15 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
receptor selective antagonists for treatment of asthma, diabetes, tumors, and other A2b assocd. diseases)

RN 552870-45-8 CAPLUS
CN Ethanediamide, N2-[6-[[2-(acetylamino)ethyl]amino]-2-phenyl-4-pyrimidinyl]-N1-(2-cyanoethyl)-N1-methyl- (CA INDEX NAME)



L15 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:573950 CAPLUS
DOCUMENT NUMBER: 125:300953
ORIGINAL REFERENCE NO.: 125:56331a,56334a
TITLE: Reaction of 3-cyano-2-methyl-1-phenylisothiourea with isocyanate, isothiocyanate and carbodiimide
AUTHOR(S): Suyama, Takayuki; Kimura, Akifumi; Kiuchi, Yasuyuki
CORPORATE SOURCE: Faculty Engineering, Kanagawa Institute Technology, Atsugi, 243-02, Japan
SOURCE: Nippon Kagaku Kaishi (1996), (9), 845-848
CODEN: NKAKB8; ISSN: 0369-4577
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB It was clarified that 3-cyano-2-methyl-1-phenylisothiourea (I) reacted with silver nitrate in the presence of triethylamine to give rise to N-cyano-N'-phenylcarbodiimide, which reacted with I to give 2-cyanoimino-4-[(N2-cyano-N1-phenylamidino)imino]-6-methylthio-1,3-diphenyl-1,2,3,4-tetrahydro-1,3,5-triazine. In a similar manner, I reacted with two molar amts. of Ph isocyanate, Ph isothiocyanate and diphenylcarbodiimide in the presence of triethylamine to afford corresponding tetrahydro-1,3,5-triazines.
IT 182944-90-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reaction of 3-cyano-2-methyl-1-phenylisothiourea with silver nitrate)
RN 182944-90-7 CAPLUS
CN Urea, N'-cyano-N-[6-(cyanoamino)-4,5-dihydro-5-phenyl-4-(phenylimino)-1,3,5-triazin-2-yl]-N-phenyl- (9CI) (CA INDEX NAME)



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CA SUBSCRIBER PRICE                                      -3.20      -4.80

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provided by InfoChem.

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DICTIONARY FILE UPDATES:  17 OCT 2008  HIGHEST RN 1062752-24-2

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on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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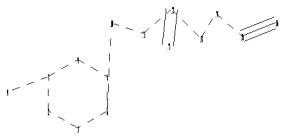

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ring bonds :
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exact/norm bonds :
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15-16

G1:C,N

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 9:CLASS 10:CLASS 11:CLASS
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L16 HAS NO ANSWERS

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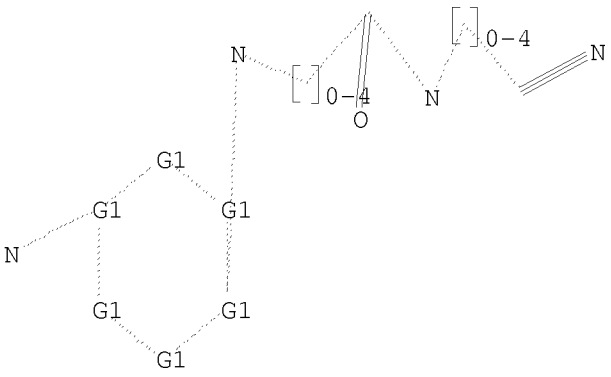

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INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
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PROJECTED ANSWERS:                2 TO      234

L17           2 SEA SSS SAM L16

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=> s l18 not l19
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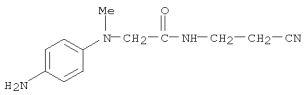
L20 ANSWER 1 OF 13 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1039831-06-5 REGISTRY
ED Entered STN: 10 Aug 2008
CN Acetamide, 2-[(4-aminophenyl)methylamino]-N-(2-cyanoethyl)- (CA INDEX NAME)
MF C12 H16 N4 O
SR Chemical Catalog
Supplier: UkrOrgSynthesis
LC STN Files: CHEMCATS



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L20 ANSWER 2 OF 13 REGISTRY COPYRIGHT 2008 ACS on STN
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SR Chemical Catalog
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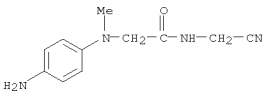
LC STN Files: CHEMCATS



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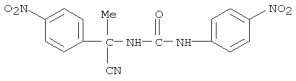

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L20 ANSWER 4 OF 13 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1022254-76-7 REGISTRY
ED Entered STN: 25 May 2008
CN Urea, N-(2-cyanoethyl)-N'-[4-(dimethylamino)phenyl]-N-[(tetrahydro-2-furanyl)methyl]- (CA INDEX NAME)
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SR Other Sources
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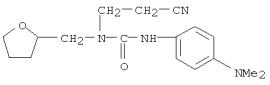

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L20 ANSWER 5 OF 13 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1020981-63-8 REGISTRY
ED Entered STN: 15 May 2008
CN Acetamide, 2-[[4-(acetylamino)phenyl]amino]-N-(cyanomethyl)- (CA INDEX NAME)
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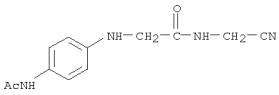
SR Chemical Catalog
Supplier: Aurora Fine Chemicals
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L20 ANSWER 6 OF 13 REGISTRY COPYRIGHT 2008 ACS on STN
RN 1020965-61-0 REGISTRY
ED Entered STN: 15 May 2008
CN Acetamide, 2-[[4-(acetylamino)phenyl]amino]-N-(2-cyanoethyl)- (CA INDEX NAME)
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SR Chemical Catalog
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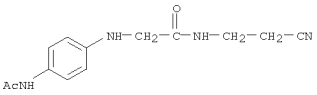
LC STN Files: CHEMCATS



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RN 909073-22-9 REGISTRY
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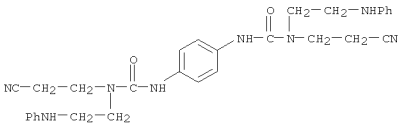

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L20 ANSWER 8 OF 13 REGISTRY COPYRIGHT 2008 ACS on STN
RN 907959-68-6 REGISTRY
ED Entered STN: 20 Sep 2006
CN INDEX NAME NOT YET ASSIGNED
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SR Other Sources
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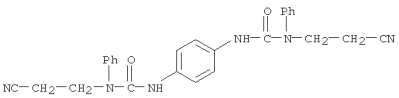

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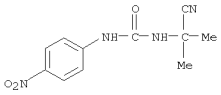
L20 ANSWER 9 OF 13 REGISTRY COPYRIGHT 2008 ACS on STN
RN 860275-17-8 REGISTRY
ED Entered STN: 15 Aug 2005
CN Urea, N-(1-cyano-1-methylethyl)-N'-(4-nitrophenyl)- (CA INDEX NAME)
MF C11 H12 N4 O3
SR Chemical Library
Supplier: AKos Consulting and Solutions GmbH
LC STN Files: CHEMCATS



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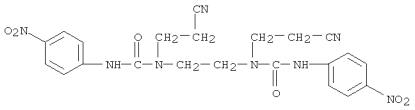
L20 ANSWER 10 OF 13 REGISTRY COPYRIGHT 2008 ACS on STN
RN 380332-15-0 REGISTRY
ED Entered STN: 03 Jan 2002
CN Urea, N,N''-1,2-ethanediylbis[N-(2-cyanoethyl)-N'-(4-nitrophenyl)- (9CI) (CA INDEX NAME)
MF C22 H22 N8 O6
SR Chemical Library
Supplier: Ambinter
LC STN Files: CHEMCATS



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L20 ANSWER 11 OF 13 REGISTRY COPYRIGHT 2008 ACS on STN
RN 294854-09-4 REGISTRY
ED Entered STN: 12 Oct 2000
CN Urea, N-(2-cyano-1,1-dimethylethyl)-N'-(4-nitrophenyl)- (CA INDEX NAME)
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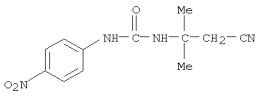
SR Chemical Library
Supplier: Oak Samples Ltd.
LC STN Files: CHEMCATS



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L20 ANSWER 12 OF 13 REGISTRY COPYRIGHT 2008 ACS on STN
RN 291278-61-0 REGISTRY
ED Entered STN: 27 Sep 2000
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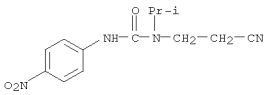
MF C13 H16 N4 O3
SR Chemical Library
Supplier: ComGenex International Inc.
LC STN Files: CHEMCATS



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L20 ANSWER 13 OF 13 REGISTRY COPYRIGHT 2008 ACS on STN
RN 289059-79-6 REGISTRY
ED Entered STN: 14 Sep 2000
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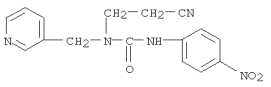
LC STN Files: CHEMCATS



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FILE COVERS 1907 - 20 Oct 2008  VOL 149 ISS 17
FILE LAST UPDATED: 19 Oct 2008  (20081019/ED)

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L3          11 S L1 FULL
L4           1 S L3 AND CAPLUS/LC
L5          10 S L3 NOT L4

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L8           2 S L7
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L10            STRUCTURE UPLOADED
L11         30 S L10 FULL SUB=L9
L12         46 S L9 NOT L11
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L13          37 S L12 AND CAPLUS/LC
L14           9 S L12 NOT L13

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     FILE 'CAPLUS' ENTERED AT 08:14:29 ON 20 OCT 2008

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L21         18 L19

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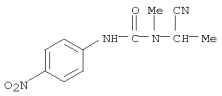
L21 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:256322 CAPLUS
DOCUMENT NUMBER: 148:517176
TITLE: Autoxidation of a 4-iminoimidazolidin-2-one with a tertiary 5-hydrogen to its 5-hydroxy derivative
AUTHOR(S): Angelova, Violina T.; Vassilev, Nikolay G.; Chauvin, Anne-Sophie; Koedjikov, Asen H.; Ivanov, Petko M.; Pojarlieff, Ivan G.
CORPORATE SOURCE: Faculty of Pharmacy, Medical University, Sofia, Bulg.
SOURCE: ARKIVOC (Gainesville, FL, United States) (2008), (11), 11-23
CODEN: AGFUAR
URL: http://content.arkat-usa.org/ARKIVOC/JOURNAL_CONTENT/manuscripts/2008/08-2730FP%20as%20published%20mainmanuscript.pdf
PUBLISHER: Arkat USA Inc.
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
AB Chemoselective autoxidn. of 4-imino-1,5-dimethyl-3-(4-nitrophenyl)imidazolidin-2-one (1b) to its 5-hydroxy derivative 2 occurred in solns. of DMSO-d6, acetonitrile-d3 or refluxing ethanol. Also bis(imidazolidin-5-yl) peroxide 5 was isolated as a minor product. It crystallizes as a 1:1 mixture of R*, R* and R*, S* diastereomers, whereas the NMR spectra of the reaction solution in DMSO-d6 showed unequal amts. of the two isomers. Mol. mechanics modeling studies with the MM3 force field indicate the R*,S* diastereomer as the more stable one. The 5-unsubstituted and the 5,5-di-Me substituted imines 1a and 1c, resp., were found stable against autoxidn.; the difference in reactivity of 1b is attributed to the single 5-Me group enhancing the population of the enamine tautomer. The 5-hydroxy-4-imino-1,5-dimethylimidazolidin-2-one (2) underwent acid hydrolysis to form 5-hydroxyhydantoin 4.
IT 700841-58-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization; autoxidn. of 4-iminoimidazolidin-2-one with tertiary 5-hydrogen to its 5-hydroxy derivative)
RN 700841-58-3 CAPLUS
CN Urea, N-(1-cyanoethyl)-N-methyl-N'-(4-nitrophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:299335 CAPLUS
DOCUMENT NUMBER: 144:350543
TITLE: Preparation of indole derivatives as inhibitors of interaction between MDM2 and p53
INVENTOR(S): Lacrampe, Jean Fernand Armand; Meyer, Christophe; Ligny, Yannick Aime Eddy; Csoka, Imre Christian Francis; Van Hijfte, Luc; Arts, Janine; Schoentjes, Bruno; Wermuth, Camille Georges; Giethlen, Bruno; Contreras, Jean-Marie; Joubert, Muriel
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 132 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006032631	A1	20060330	WO 2005-EP54604	20050916
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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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EP 1809622	A1	20070725	EP 2005-786991	20050916
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KR 2007058622	A	20070608	KR 2007-708663	20070417

PRIORITY APPLN. INFO.: EP 2004-77630 A 20040922
US 2004-613902P P 20040928
WO 2005-EP54604 W 20050916

OTHER SOURCE(S): MARPAT 144:350543
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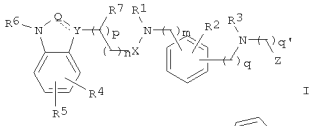
L21 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



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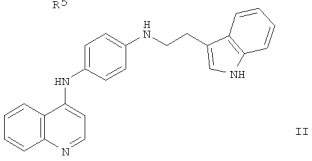
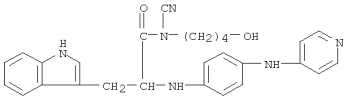


II

AB The title compds. I [wherein m = 0-2; n = 0-3; p, q and q' = independently 0 or 1; X = CO or (un)substituted CH2; Q-Y = (un)substituted CH=C, CO-CH, CO-N, CH2-CH, or CH2-N; R1 = H, aryl, heteroaryl, alkyl, etc.; R2 = H, halo, alkyl, alkoxy, etc.; R3 = H, alkyl, heteroaryl, etc.; R4 and R5 = independently H, halo, alkyl, CN, etc.; R6 = H, alkoxycarbonyl, or alkyl; Z = (un)substituted heteroaryl; with provisos] or N-oxides, salts, or stereoisomers thereof are prepared as inhibitors of interaction between MDM2 and p53. For example, the compound II•xHCl was prepared in a multi-step synthesis. I showed inhibitory effect on cell proliferation. Formulations containing I as an active ingredient were also described.
IT 881204-17-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of indole derivs. as inhibitors of interaction between MDM2 and p53)
RN 881204-17-7 CAPLUS
CN 1H-Indole-3-propanamide, N-cyano-N-(4-hydroxybutyl)-α-[[4-(4-pyridinylamino)phenyl]amino]- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

L21 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1242315 CAPLUS
DOCUMENT NUMBER: 143:477661
TITLE: Preparation of cyclohexyldiamine derivatives as modulators of ORL1 receptors
INVENTOR(S): Sundermann, Corinna; Sundermann, Bernd
PATENT ASSIGNEE(S): Gruenenthal G.m.b.H., Germany
SOURCE: PCT Int. Appl., 93 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

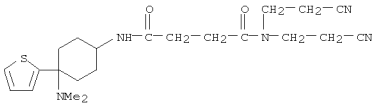
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005110974	A1	20051124	WO 2005-EP4913	20050506
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 102004023522	A1	20051201	DE 2004-102004023522	20040510
CA 2566297	A1	20051124	CA 2005-2566297	20050506
EP 1745010	A1	20070124	EP 2005-739598	20050506
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, LV				
JP 2007536323	T	20071213	JP 2007-512033	20050506
US 20070112007	A1	20070517	US 2006-594963	20061109
PRIORITY APPLN. INFO.:			DE 2004-102004023522A	20040510
			WO 2005-EP4913 W	20050506

OTHER SOURCE(S): MARPAT 143:477661
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

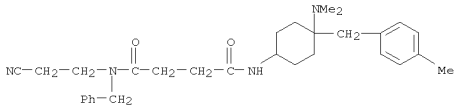
AB Title compds. I [n = 1-5; R1 and R2 independently = H, (un)substituted alkyl, cycloalkyl, etc. or R1 and R2 together may form CH2CH2OCH2CH2, CH2CH2NR6CH2CH2 or (CH2)3-6; R6 = H, (un)substituted alkyl, aryl, etc.; R3 = (un)substituted alkyl, cycloalkyl, heteroaryl, etc.; R4 = -(CR7R8)pR9; p = 0-4; R7 = H or (un)substituted alkyl; R8 = H, (un)substituted alkyl and COOR10 or R7 and R8 together may form ring (CH2)yCHR9(CH2)m; y = 1-3; m = 1-2; R9 = (un)substituted alkyl, aryl, heteroaryl, etc.; R10 = H or alkyl; R5 = H or -(CH2)xR9 or together with R4 may form CH2CHR11OCHR11CH2, CH2CH2SCH2CH2, CH2CH2NR12CH2CH2, etc.; R11 = H or (un)substituted alkyl;

L21 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

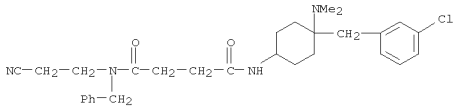


REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
R12 = H, (un)substituted alkyl, cycloalkyl, etc.; x = 1-3] and their pharmaceutically acceptable salts, are prepd. and disclosed as modulators of ORL1 receptors. Thus, e.g., II was prepd. by coupling of 4-[2-(4-chlorophenyl)ethyl-carbamoyl]butyric acid with 4-benzyl-4-dimethylaminocyclohexanone and subsequent conversion into the hydrochloride. The binding activity of I towards ORL1 receptors was evaluated in scintillation assays using recombinant CHO-ORL1 cells and it was revealed that selected compds. of the invention displayed binding activity in the range of 39 up to 100%. I as modulator of ORL1 receptors should prove useful in the treatment of obesity, depression and pain. Pharmaceutical compns. comprising I are disclosed.
IT 869745-13-1P 869745-41-5P 869746-27-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclohexyldiamine derivs. as modulators of ORL1 receptors)
RN 869745-13-1 CAPLUS
CN Butanediamide, N1-(2-cyanoethyl)-N4-[4-(dimethylamino)-4-[(4-methylphenyl)methyl]cyclohexyl]-N1-(phenylmethyl)- (CA INDEX NAME)



RN 869745-41-5 CAPLUS
CN Butanediamide, N4-[4-[(3-chlorophenyl)methyl]-4-(dimethylamino)cyclohexyl]-N1-(2-cyanoethyl)-N1-(phenylmethyl)- (CA INDEX NAME)



RN 869746-27-0 CAPLUS
CN Butanediamide, N1,N1-bis(2-cyanoethyl)-N4-[4-(dimethylamino)-4-(2-thienyl)cyclohexyl]- (CA INDEX NAME)

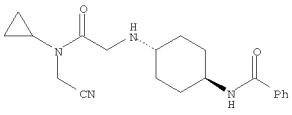
L21 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:259865 CAPLUS
DOCUMENT NUMBER: 142:336644
TITLE: Preparation of amino acid derivatives as dipeptidyl peptidase IV inhibitors
INVENTOR(S): Tsutsumi, Kazuhiro; Shinkai, Hisashi; Kitao, Yuki; Yamashita, Masaki; Kobayashi, Satoru; Matsui, Kenichi; Oda, Tomohiro; Taniguchi, Toshio; Asahina, Kota
PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
SOURCE: PCT Int. Appl., 356 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005025554	A2	20050324	WO 2004-JP13480	20040909
WO 2005025554	A3	20050728		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			JP 2003-317407	A 20030909
			JP 2003-395879	A 20031126
			JP 2004-114685	A 20040408

OTHER SOURCE(S): CASREACT 142:336644; MARPAT 142:336644
AB The invention relates to amino acid amides R1NHCR4R5CONR2R3 [R1, R2 = H, (un)substituted alkyl or cycloalkyl; R3 = (un)substituted alkyl or cycloalkyl; R4, R5 = H, (un)substituted alkyl, cycloalkyl, aryl, aralkyl, heterocyclyl or heterocyclylalkyl], including stereoisomers or pharmaceutically-acceptable salts, which show dipeptidyl peptidase IV (DPP-IV) inhibitory activity and are effective for the treatment of type II diabetes, obesity, etc. Thus, (2S)-N-cyclobutyl-N-methyl-2-amino-2-cyclohexylacetamide hydrochloride, prepared by amidation reaction, showed IC50 < 10 μM for inhibition of DPP-IV.
IT 848494-03-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid derivs. as dipeptidyl peptidase IV inhibitors)
RN 848494-03-1 CAPLUS
CN Benzamide, N-[trans-4-[[2-[(cyanomethyl)cyclopropylamino]-2-oxoethyl]amino]cyclohexyl]- (CA INDEX NAME)

Relative stereochemistry.

L21 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



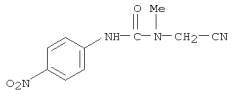
L21 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:187090 CAPLUS
DOCUMENT NUMBER: 141:23150
TITLE: Synthesis of 4-imino-1-methyl-3-(4-nitrophenyl)imidazolidin-2-ones; pK-values, E,Z-isomerism and exchange of the imino proton
AUTHOR(S): Angelova, V. T.; Vasilev, N. G.; Koedjikov, A. H.; Pojarlieff, I. G.
CORPORATE SOURCE: Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, Sofia, 1113, Bulg.
SOURCE: Bulgarian Chemical Communications (2003), 35(2), 122-128
CODEN: BCHCE4; ISSN: 0324-1130
PUBLISHER: Bulgarian Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:23150

AB The preparation of 4-imino-1-methyl-3-(4-nitrophenyl)imidazolidin-2-one (Im-1) and its 5-methyl- and 5,5'-dimethyl- derivs. (Im-2 and Im-3) is reported via the resp. ureido nitriles from methylaminonitriles and 4-nitrophenyl isocyanate. The pKBH+ of the imines were determined spectrophotometrically in aqueous buffers, Im-1 being the strongest base. The 1H NMR spectra of the imines show E,Z-isomers around the C=N bond, the major isomer assigned as E. Depending upon the solvent, the concentration and the temperature various states of exchange on the NMR scale were observed The broadening of the signals of the Ph o-protons is characteristic. Two dimensional 1H NMR EXSY in DMSO-d6 indicated exchange of protons between the configurational isomers and water. The rates of exchange between the three sites were determined by the 2DNMR program. Im-3 exchanges faster than Im-1. The slow E,Z-isomerization on the NMR time-scale of C=NH imines is especially unusual due to fast intermol. proton exchange. Its exhibition in the NMR spectra in the case studied is attributed to the lower basicity of the iminoimidazolidinones slowing down proton transfer.

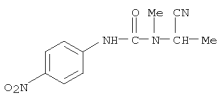
IT 5594-49-0P 700841-58-3P 700841-60-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, pK-values, E,Z-isomerism and exchange of imino proton of 4-imino-1-methyl-3-(4-nitrophenyl)imidazolidin-2-ones)

RN 5594-49-0 CAPLUS
CN Urea, N-(cyanomethyl)-N-methyl-N'-(4-nitrophenyl)- (CA INDEX NAME)

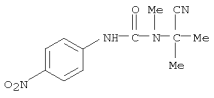


RN 700841-58-3 CAPLUS
CN Urea, N-(1-cyanoethyl)-N-methyl-N'-(4-nitrophenyl)- (CA INDEX NAME)

L21 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 700841-60-7 CAPLUS
CN Urea, N-(1-cyano-1-methylethyl)-N-methyl-N'-(4-nitrophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

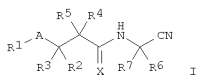
L21 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:833854 CAPLUS
DOCUMENT NUMBER: 135:371749
TITLE: Preparation of succinic acid diamides as cysteine protease inhibitors
INVENTOR(S): Bekkali, Younes; Betageri, Rajashehar; Emmanuel, Michel Jose; Hickey, Eugene Richard; Liu, Weimin; Patel, Usha R.; Spero, Denice Mary; Thomson, David S.; Ward, Yancey David; Young, Erick Richard Roush
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 75 pp., Cont.-in-part of U.S. Ser. No. 627,869.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20010041700	A1	20011115	US 2001-862674	20010522
US 6313117	B1	20011106	US 2000-627869	20000728
US 20030087939	A1	20030508	US 2002-278546	20021023
US 6649642	B2	20031118		

PRIORITY APPLN. INFO.: US 1999-146647P P 19990730
US 2000-627869 A2 20000728
US 2001-862674 A1 20010522

OTHER SOURCE(S): MARPAT 135:371749
GI



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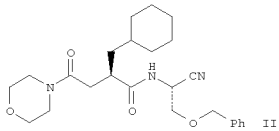


II

AB Title compds. [I; A = CO, R8OCH; R1 = (substituted) alkyl, cycloalkyl, aryl, heterocyclyl, heteroaryl, amino; R2 = H, alkyl, OH, alkoxy; R3, R4 =

L21 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

H, alkyl; R5 = H, alkyl, cycloalkyl, aryl, heterocyclyl, heteroaryl; R6 = H, alkyl optionally interrupted by 1-2 N, O, S; R7 = H, alkyl, alkyl interrupted by 1-2 N, O, S, cycloalkyl, aryl, heterocyclyl, aryl, heteroaryl, cyano; R6R7 = atoms to form a 4-7 membered heterocyclic or carbocyclic ring; R8 = H, alkyl, cycloalkyl, cycloalkylalkyl, aralkyl; X = O, S], were prepd. as inhibitors of cysteine proteases such as cathepsins B, F, K, L, and S in the treatment of autoimmune diseases, Alzheimer's disease, and atherosclerosis. Thus, (R)-2-cyclohexylmethyl-4-morpholin-4-yl-4-oxobutyric acid (prepn. given) in DMF at 0° was treated with EDC, 1-hydroxybenzotriazole, O-benzyl-L-serinamide.HCl, and N-methylmorpholine followed by stirring overnight to give N-(2-benzyloxy-1-carbamoylethyl)-2-cyclohexylmethyl-4-morpholin-4-yloxobutyramide. The latter was stirred 1 h with cyanuric chloride in DMF at 0° to give title compd. (II). I inhibited cathepsin S with IC50≤ 100 μM.

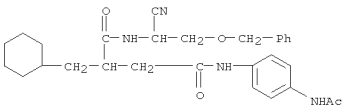
IT 324794-60-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of succinic acid diamides as inhibitors of cysteine proteases (cathepsins) in the treatment of autoimmune diseases, Alzheimer's disease, and atherosclerosis)

RN 324794-60-7 CAPLUS

CN Butanediamide, N4-[4-(acetylamino)phenyl]-N1-[1-cyano-2-(phenylmethoxy)ethyl]-2-(cyclohexylmethyl)- (CA INDEX NAME)



L21 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:101117 CAPLUS

DOCUMENT NUMBER: 134:163044

TITLE: Preparation of succinic acid diamides as cysteine protease inhibitors

INVENTOR(S): Bekkali, Younes; Betageri, Raj; Emmanuel, Michel; Hickey, Eugene; Liu, Weimin; Spero, Denice M.; Thomson, David S.; Ward, Yancey; Young, Erick R. R.; Patel, Usha

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 221 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001009110	A1	20010208	WO 2000-US20453	20000728
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2379747	A1	20010208	CA 2000-2379747	20000728
CA 2379747	C	20080923		
EP 1204652	A1	20020515	EP 2000-950777	20000728
EP 1204652	B1	20060517		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003506364	T	20030218	JP 2001-514313	20000728
AT 326454	T	20060615	AT 2000-950777	20000728
ES 2264937	T3	20070201	ES 2000-950777	20000728
MX 2002PA01014	A	20020812	MX 2002-PA1014	20020129

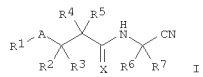
PRIORITY APPLN. INFO.: US 1999-146647P P 19990730

WO 2000-US20453 W 20000728

OTHER SOURCE(S): MARPAT 134:163044

GI

L21 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



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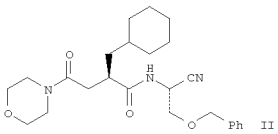


II

AB Title compds. [I; A = CO, R8OCH; R1 = (substituted) alkyl, cycloalkyl, aryl, heterocyclyl, heteroaryl, amino; R2 = H, alkyl, OH, alkoxy; R3, R4 = H, alkyl; R5 = H, alkyl, cycloalkyl, aryl, heterocyclyl, heteroaryl; R6 = H, alkyl optionally interrupted by 1-2 N, O, S; R7 = H, alkyl, alkyl interrupted by 1-2 N, O, S, cycloalkyl, aryl, heterocyclyl, aryl, heteroaryl, cyano; R6R7 = atoms to form a 4-7 membered heterocyclic or carbocyclic ring; R8 = H, alkyl, cycloalkyl, cycloalkylalkyl, aralkyl; X = O, S], were prepared *s* inhibitors of cysteine proteases such as cathepsins B, F, K, L, and S in the treatment of autoimmune diseases, Alzheimer's disease, and atherosclerosis. Thus, (R)-2-cyclohexylmethyl-4-morpholin-4-yl-4-oxobutyric acid (preparation given) in DMF at 0° was treated with EDC, 1-hydroxybenzotriazole, O-benzyl-L-serinamide, and N-methylmorpholine followed by stirring overnight to give N-(2-benzyloxy-1-carbamoylethyl)-2-cyclohexylmethyl-4-morpholin-4-yloxobutyramide. The latter was stirred 1 h with cyanuric chloride in DMF at 0° to give title compound (II). I inhibited cathepsin S with IC50≤ 100 μM.

IT 324794-60-7P

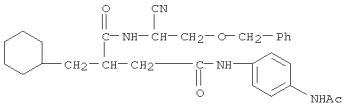
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of succinic acid diamides as inhibitors of cysteine proteases (cathepsins) in the treatment of autoimmune diseases, Alzheimer's disease, and atherosclerosis)

RN 324794-60-7 CAPLUS

CN Butanediamide, N4-[4-(acetylamino)phenyl]-N1-[1-cyano-2-(phenylmethoxy)ethyl]-2-(cyclohexylmethyl)- (CA INDEX NAME)

L21 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

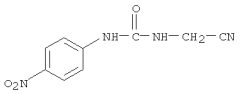


REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 8 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:651417 CAPLUS
DOCUMENT NUMBER: 133:321154
TITLE: Structure-activity relationship of sweet molecules: phenylurea derivatives
AUTHOR(S): Jasiczak, J.; Jonska-Muteba, E.; Zalewski, R. I.
CORPORATE SOURCE: Department of Chemistry of Natural Products, Poznan University of Economics, Poznan, 60 967, Pol.
SOURCE: Polish Journal of Chemistry (2000), 74(9), 1259-1273
CODEN: PJCHDQ; ISSN: 0137-5083
PUBLISHER: Polish Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

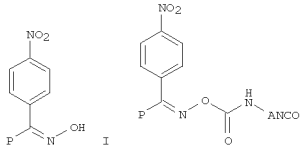
AB A model of sweet and non-sweet substituted phenylureas has been developed by discriminant anal. of chemical and structural data. The model has been used to predict the taste of addnl. phenylurea derivs. of unknown taste and to select candidates for chemical synthesis and sensory anal. The 3-dimensional computer aided model of compds. of interest was generated and fitted a spatial receptor model, to discuss importance of hydrogen bonding, bulkiness and the steric factor for sweetness.

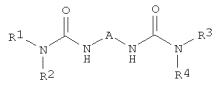
IT 302896-85-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(structure-activity relationship of sweet mols., phenylurea derivs.)
RN 302896-85-1 CAPLUS
CN Urea, N-(cyanomethyl)-N'-(4-nitrophenyl)- (CA INDEX NAME)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:683459 CAPLUS
DOCUMENT NUMBER: 126:74337
ORIGINAL REFERENCE NO.: 126:14389a
TITLE: Diisocyanates as scaffolds for combinatorial libraries. The solid-phase synthesis of bis[ureas] from polymer-supported diisocyanates
AUTHOR(S): Scialdone, Mark A.
CORPORATE SOURCE: Central Res. and Development, E. I. Du Pont de Nemours and Co., Wilmington, DE, 19880-0328, USA
SOURCE: Tetrahedron Letters (1996), 37(45), 8141-8144
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

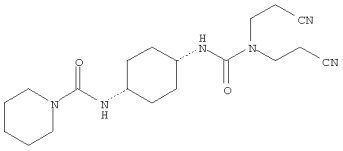




AB A general method for preparation of bis[ureas] was developed from oxime resin-derived carbamates of diisocyanates. Thus, monoaddn. of diisocyanates a polymer-supported 4-nitrobenzaldehyde oxime I (P = polymer support) gave isocyanates II (P = polymer support; A = alkanediyl). Treatment of II with amines gave the alkanediylbis[ureas] III (R1-R4 = alkyl, cyclohexylmethyl, 4-morpholinyl, etc.). Directional urea synthesis was achieved by sequential amine addition which demonstrated the utility of thermolabile oxime-derived carbamate linkages to a polymer support. The products, obtained in good yield in three steps, were of high chemical purity.

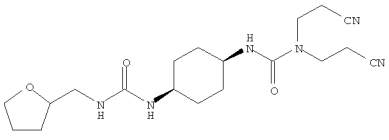
IT 185433-06-1P 185433-07-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of alkanediylbis[ureas] from polymer-supported diisocyanates)
RN 185433-06-1 CAPLUS
CN 1-Piperidinecarboxamide, N-[cis-4-[[[bis(2-cyanoethyl)amino]carbonyl]amino]cyclohexyl]- (CA INDEX NAME)

L21 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
Relative stereochemistry.



RN 185433-07-2 CAPLUS
CN Urea, N,N-bis(2-cyanoethyl)-N'-[4-[[[[(tetrahydro-2-furanyl)methyl]amino]carbonyl]amino]cyclohexyl]-, cis- (9CI) (CA INDEX NAME)

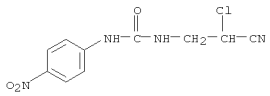
Relative stereochemistry.



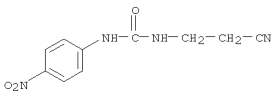
L21 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1980:514106 CAPLUS
DOCUMENT NUMBER: 93:114106
ORIGINAL REFERENCE NO.: 93:18249a,18252a
TITLE: Reactivity of N,N-dichlorourethanes. IX. Addition of N,N-dichlorourethanes to alkenes with electron-acceptor groups
AUTHOR(S): Balon, Ya. G.; Paranyuk, V. E.
CORPORATE SOURCE: Kiev. Nauchno-Issled. Inst. Endokrinol. Obmena Veshchestva, Kiev, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1980), 16(3), 556-63
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 93:114106

AB Addition of Cl2NCO2R (R = Me, Et) to R1CH:CH2 (R1 = cyano, MeO2C, H2NCO) in the presence of powdered Cu or CuCl gave 4 corresponding R1CHClCH2NClCO2R (I) in 58-83% yield. Treating I with Na2SO3 or Na2S2O3 yielded 77-94% R1CHClCH2NHCO2R (II) which cyclized at 160-70° to give 41% 5-cyano- and 32% 5-(methoxycarbonyl)oxazolidin-2-one. I (R = Me, Et; R1 = cyano) reacted with P(OEt)3 in refluxing C6H6 to give 64-7% NCCHClCH2N(CO2R)P(O)(OEt)2 (same R) and 87-90% EtCl, and pyrocatechol trichlorophosphate to give 67% NCCHClCH2NCO (III). III reacted with ROH (R = Me, Et) to give II (same R, R1 = cyano), with H2O to give 63% (NCCHClCH2NH)2CO, and p-R2C6H4NH2 (R2 = H, Me, MeO, Cl, Br, iodo, O2N) to give the corresponding NCCHClCH2NHCONHC6H4R2-p (IV) in 78-92% yield. Reactions of IV are described.

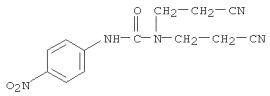
IT 74448-71-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 74448-71-8 CAPLUS
CN Urea, N-(2-chloro-2-cyanoethyl)-N'-(4-nitrophenyl)- (CA INDEX NAME)



L21 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1980:462587 CAPLUS
DOCUMENT NUMBER: 93:62587
ORIGINAL REFERENCE NO.: 93:10127a,10130a
TITLE: Sweet taste receptor. Evidence of separate specific sites for carboxyl ion and nitrite/cyanide groups in sweeteners
AUTHOR(S): Tinti, J. M.; Durozard, D.; Nofre, C.
CORPORATE SOURCE: Lab. Biochim. Struct., Fac. Med. Alexis-Carrel, Lyon, Fr.
SOURCE: Naturwissenschaften (1980), 67(4), 193-4
CODEN: NATWAY; ISSN: 0028-1042
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In tests of 16 compds., the NO2 and CN groups in sweeteners acted on sweet
taste receptors similarly, and both acted differently from the COO- groups. The sweet taste receptor may have 2 specific sites, 1 for the NO2
and CN groups, and 1 for the COO- group.
IT 74390-17-3
RL: PRP (Properties)
(sweetness taste receptor response to)
RN 74390-17-3 CAPLUS
CN Urea, N-(2-cyanoethyl)-N'-(4-nitrophenyl)- (CA INDEX NAME)



L21 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:512522 CAPLUS
DOCUMENT NUMBER: 71:112522
ORIGINAL REFERENCE NO.: 71:20919a,20922a
TITLE: Reaction of 1,1-bis(β-cyanoethyl)urea with aromatic amines
AUTHOR(S): Kretov, A. E.; Borodavko, N. D.; Gaponova, A. P.
CORPORATE SOURCE: Dnepropetrovsk. Khim.-Tekhnol. Inst., Dnepropetrovsk, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1969), 5(8), 1466-9
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB The reaction of H2NCON(CH2CH2CN)2 with aromatic primary amines gave mixts.
of NH(CH2CH2CN)2, RNHCONHR (I), and RNHCON(CH2CH2CN)2 (II) (R is Ph, 4-MeC6H4, 2-MeC6H4, 3-MeC6H4, 3,4-ClMeC6H3, 4-O2NC6H4, 3-O2NC6H4, 2,4-Cl2C6H3, or 4-Et-OC6H4). The relative amts. of I and II depended on the reaction conditions. Heating II in EtOH containing NaOH gave RNHCONH2 and
EtOCH2CH2CN. Refluxing I (R = p-Me-C6H4) in concentrate HCl solution gave NH4Cl
and 1-(β-carboxyethyl)-2,4-dioxo-3-(p-tolyl)hexahydropyrimidine.
IT 23993-79-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23993-79-5 CAPLUS
CN Urea, 1,1-bis(2-cyanoethyl)-3-(p-nitrophenyl)- (8CI) (CA INDEX NAME)

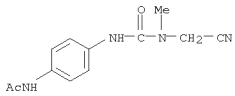


L21 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:18945 CAPLUS
DOCUMENT NUMBER: 64:18945
ORIGINAL REFERENCE NO.: 64:3417c-f
TITLE: 1,3-Substituted ureas as selective herbicides
INVENTOR(S): Simonian, John V.; Kroll, Harry; Peterson, Janet B.
PATENT ASSIGNEE(S): Geigy Chemical Corp.
SOURCE: 5 pp.; Division of U.S. 3,134,663 (CA 61, 3117c)
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

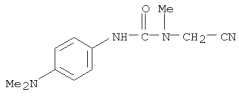
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3205258		19650907	US 1958-751589	19580714
PRIORITY APPLN. INFO.:			US	19580714

GI For diagram(s), see printed CA Issue.
AB Ia can be formulated into compns. to provide selective control of weeds, without imparting to the soil long-lasting herbicidal properties.
3-(2,4-Dichlorophenyl)-1-methyl-1-cyanomethylurea is prepared by treating 57
parts 2,4-dichlorophenyl isocyanate in 130 parts dry C6H6 with a solution of
21 parts N-methylamino-acetonitrile in 150 parts of dry C6H6 at 40-50° for 1.5 hrs.; total yield is 70%, m. 120-6:
3-(3-trifluoromethyl-4-chlorophenyl)-1-methyl-1-cyanomethylurea is prepared
by treating a solution of 54.7 parts of 3-trifluoromethyl-4-chloroaniline and
22.1 parts pyridine in 145 parts C6H6 with a solution of 37.1 parts N-methyl-N-cyanomethylcarbamoyl chloride in 44 parts C6H6 at 40-50° for 2 hrs.; yield is 89%, m. 139-43°. Similarly are prepared the following 3-substituted 1-methyl-1-cyanomethylureas [3-substituent(s), % yield, and m.p. given]: o-ClC6H4, --, 87.5-8.5°; p-ClC6H4, 90, 92-6°; m-ClC6H4, --, 96.5-8.5°; 3,4-Cl2C6H3, 99, 104-7°, 2,4,5-Cl3C6H2, 75, --; m-tolyl, 63, --; p-tolyl, 94.5, 120-8°, 3,4-Me2C6H3, 91, 153-5°; p-MeOC6H4, 92.5, 104-12°; 2,5-(MeO)2C6H3, 86, 136-41°; Ph, Me, 83, --; p-AcNHC6H4, 80.5, 176-7° (evolution of gas); p-Me2NC6H4, 72, 122-4.5°; p-FC6H4, 89, 127-9°. Also prepared are 3-(p-chlorophenyl)-1-sec-propyl-1-cyanomethylurea, m. 88-96°; 3-(3,4-dichlorophenyl)-1-sec-propyl-1-cyanomethylurea; 79.5% 3-(2,4-dichlorophenyl)-1-methyl-1-carbethoxymethylurea, m. 59-60.5°; 90.5% 3-(p-chlorophenyl)-1-methyl-1-carbethoxymethylurea, m. 115.5-18°; 86% 3-(2,5-dichlorophenyl)-1-methyl-1-carbethoxymethylurea, m. 81-2°; 33% 3-(o-chlorophenyl)-1-methyl-1-carbethoxymethylurea; and 93% 3-(p-chlorophenyl)-1-methyl-1-carboxymethylurea, m. 127-8.5° (evolution of gas).
IT 4954-36-3P, Urea, 3-(p-acetamidophenyl)-1-(cyanomethyl)-1-methyl- 4954-37-4P, Urea, 1-(cyanomethyl)-3-[p-(dimethylamino)phenyl]-1-methyl- 5594-49-0P, Urea, 1-(cyanomethyl)-1-methyl-3-(p-nitrophenyl)-
RL: PREP (Preparation)
(preparation of)
RN 4954-36-3 CAPLUS
CN Urea, 3-(p-acetamidophenyl)-1-(cyanomethyl)-1-methyl- (6CI, 7CI, 8CI) (CA

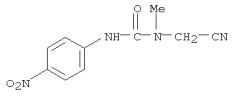
L21 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
INDEX NAME)



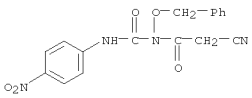
RN 4954-37-4 CAPLUS
CN Urea, 1-(cyanomethyl)-3-[p-(dimethylamino)phenyl]-1-methyl- (6CI, 8CI) (CA INDEX NAME)



RN 5594-49-0 CAPLUS
CN Urea, N-(cyanomethyl)-N-methyl-N'-(4-nitrophenyl)- (CA INDEX NAME)



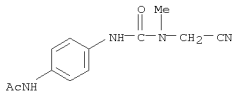
L21 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:464372 CAPLUS
DOCUMENT NUMBER: 61:64372
ORIGINAL REFERENCE NO.: 61:11187a-c
TITLE: A pharmacologic study of some hydroxamic acid esters
AUTHOR(S): Kehl, Horst
CORPORATE SOURCE: Kirksville Coll. Osteopathy & Surgery, Kirksville, MO
SOURCE: Journal of the American Osteopathic Association (1964), 63(9), 872-3
CODEN: JAOAAZ; ISSN: 0098-6151
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB A series of hydroxamic acid esters were synthesized, viz., N-cyanoacetyl-O-benzylhydroxylamine (I), N-acetyl-O-(carbomethoxymethyl)-hydroxylamine (II), N-glycol-O-benzylhydroxylamine (III), N-(carbamoylacetyl)-O-benzylhydroxylamine (H2NCCH2CNHO-CH2Ph) (IV); and N-(cyanoacetyl)-N-(p-nitrophenylcarbamoyl)-O-benzylhydroxylamine (V). III had a stimulating effect on the respiratory system and acted as a Lewis acid. IV had intermediate activity; its ability to act as a Lewis acid was reduced by its amide group. I lacked pharmacol. activity and could not act as a Broensted acid because its nitrile group stabilized the H at the methylene group. I did not react with acid chloride or an isocyanate, indicating that the H at the N was unavailable for chemical reaction. III, 0.5 g./kg. body weight, produced respiratory stimulation. A hydroxamic acid ester must apparently be able to function as a Lewis acid in order to have pharmacol. activity.
IT 93320-83-3, Urea, 1-(benzyloxy)-1-(cyanoacetyl)-3-(p-nitrophenyl)- (pharmacology of)
RN 93320-83-3 CAPLUS
CN Acetamide, 2-cyano-N-[[(4-nitrophenyl)amino]carbonyl]-N-(phenylmethoxy)- (CA INDEX NAME)



L21 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1961:114082 CAPLUS
DOCUMENT NUMBER: 55:114082
ORIGINAL REFERENCE NO.: 55:21465h-i,21466a-b
TITLE: Substituted urea herbicides
INVENTOR(S): Simonian, John Vahan; Kroll, Harry; Peterson, Janet B.
PATENT ASSIGNEE(S): J. R. Geigy Akt.-Ges.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

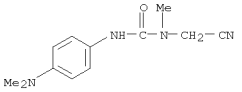
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 863443		19610322	GB 1958-23420	19580722

AB 3-Aryl-1-alkyl-1-(cyanomethyl)ureas were found to possess selective herbicidal activity. o-Chlorophenyl isocyanate (98.6 parts) in 100 parts C6H6 was added to a mixture of 45 parts sarcosinonitrile (I) in 100 parts C6H6, refluxed for 3 hrs., and cooled. Ligroine was added to turbidity, and the mixture was cooled to 10° for 24 hrs. and filtered in vacuo to yield 138 parts 3-(o-chlorophenyl)-1-methyl-1-(cyanomethyl)urea (II), m. 87.5-8.5°. Similarly prepared were the analogs of II (compound and m.p. given): 3-(p-chlorophenyl), 92-6°; 3-(m-chlorophenyl), 96.5-8.5°; 3-(3,4-dichlorophenyl), 104-7°; 3-(2,4,5-trichlorophenyl), -; 3-(2,4-dichlorophenyl), 120-6°; 3-(m-tolyl), -; 3-(p-tolyl), 120-8°; 3-(p-methoxyphenyl), 104-12°; 3-(2,5-dimethoxyphenyl), 136-41°; 3-(3-trifluoromethyl-4-chlorophenyl), 139-43°; 3-(p-acetamidophenyl), 176-7°; 3-(p-dimethylaminophenyl), 122-4.5°; and 3-(p-fluorophenyl), 127-9°. Similarly prepared were 3-(3,4-dimethylphenyl)-1-(cyanomethyl)urea, 153-5°; 3-(p-chlorophenyl)-1-isopropyl-1-(cyanomethyl)urea, 88-96°; 3-(3,4-dichlorophenyl)-1-isopropyl]-1-(cyanomethyl)urea, -; and 3-phenyl-1,3-dimethyl-1-(cyanomethyl)urea (III). N-Methyl-N-(cyanomethyl)carbamoyl chloride, b18 124-37°, n25D 1.485, was prepared from I and COCl2. III gave effective weed control at 4 lb./acre in preemergence applications.
IT 4954-36-3, Urea, 3-(p-acetamidophenyl)-1-(cyanomethyl)-1-methyl- 4954-37-4, Urea, 1-(cyanomethyl)-3-(p-dimethylaminophenyl)-1-methyl- (for weed control)
RN 4954-36-3 CAPLUS
CN Urea, 3-(p-acetamidophenyl)-1-(cyanomethyl)-1-methyl- (6CI, 7CI, 8CI) (CA INDEX NAME)



RN 4954-37-4 CAPLUS
CN Urea, 1-(cyanomethyl)-3-[p-(dimethylamino)phenyl]-1-methyl- (6CI, 8CI) (CA INDEX NAME)

L21 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



L21 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1961:17827 CAPLUS
DOCUMENT NUMBER: 55:17827
ORIGINAL REFERENCE NO.: 55:3531e-i,3532a-h
TITLE: Reformatskii reaction of the tetralones and indanones
AUTHOR(S): Ahmed, Hafez; Campbell, Neil
CORPORATE SOURCE: Univ. Edinburgh, UK
SOURCE: Journal of the Chemical Society (1960) 4115-20
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 55:17827
AB The constitutions of the unsatd. acids obtained by the interaction of BrCH2CO2Et (I) and Zn with tetralones and indanones were estimated 1-Tetralone (50 g.) added with vigorous stirring to 18 g. Zn wool, 300 ml. C6H6, and 60 g. I previously warmed to 60°, after the initial reaction subsided the mixture refluxed 1.5 hrs., the solution decanted, MeOH added to give a clear solution, dilute H2SO4 added, the aqueous solution twice extracted with C6H6, washed, and distilled gave 50 g. Et 1,2,3,4-tetrahydro-1-hydroxy-1-naphthaleneacetate (II), b10 185-90°. II (5 g.) in 20 ml. H2O and 5 ml. 40% MeOH-KOH kept 24 hrs. at room temperature, warmed 20 min. to 60°, and treated with H2O and dilute HCl gave the hydroxy acid, oil; acylurea derivative, prismatic needles, m. 172-3°. The ester (40 g.) heated 15 min. with 120 ml. anhydrous HCO2H, the excess HCO2H removed by blowing air through the hot solution, the unsatd. esters (30 g.) distilled at 190-5°/8 mm., refluxed 2 hrs. with 200 ml. 10% MeOH-KOH, most of the alc. distilled, and H2O and HCl added gave 18 g. mixed unsatd. acids, m. 84-98°. The Et2O shaken with NaHCO3 solution and evaporated gave 1.2 g. 1,2,3,4-tetrahydro-1-naphthylideneacetic acid (III), prismatic needles, m. 162-3° (ligroine); acylurea m. 176-7° (Me2CO). Ozonolysis of III yielded 1-tetralone; dinitrophenylhydrazone m. 258-9°. The aqueous layer with dilute HCl gave a mixture of acids, 10 g. of which repeatedly refluxed with 200 ml. H2O gave an oily residue, which crystallized afforded 3,4-dihydro-1-naphthaleneacetic acid (IV), prisms, m. 107° (ligroine); acylurea, prisms, m. 162-3°. IV (5 g.) refluxed with 100 ml. dilute H2SO4 gave 2.5 g. 1,2-dihydro-4-methylnaphthalene (V), b14 105-7°. V with chloranil in refluxing xylene 4 hrs. gave 1-methylnaphthalene; picrate m. 141-2°; trinitrobenzene adduct m. 154°. The ozonolysis product could not be identified. The acid (1 g.) with 15 ml. cold Et2O and Br followed by precipitation with ligroine gave the dibromide, prisms, m. 148-50° (decomposition). The 3 acids were spotted on paper. The acids, m. 106-7° and 90-2°, travelled at the same rate and gave yellow spots with a violet fluorescence in ultraviolet light. The other isomer could not be traced. This suggested that the low-melting acid was an impure sample of the acid, m. 106-7°. Tetralone (60 g.), 46.6 g. NCCH2CO2Et, 6.4 g. NH4OAc, 19 g. AcOH, and 150 ml. C6H6 heated under a H2O separator, and fractionally distilled yielded 36 g. Et α-cyano-3,4-dihydro-1-naphthalene acetate (VI), b9 202-6°. VI (2 g.) gave 1-tetralone when refluxed 6 hrs. with 50 ml. concentrated HCl or

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with 40 ml. each concd. H_2SO_4, AcOH, and H_2O and when refluxed with 5 g. NaOH in 40 ml. H_2O and 20 ml. alc. gave IV. VI (5 g.) was refluxed 3.5 hrs. with 400 ml. alc. and 400 ml. concd. HCl, 500 ml. H_2O added, the mixt. extd. with Et_2O, the exts. washed, and shaken with dil. $NaHCO_3$. The alk. layer with dil. H_2SO_4 gave α-cyano-1,2,3,4-tetrahydro-1-naphthylideneacetic acid (VII), m. 172-8° (decompn.) (aq. alc.); acylurea, yellow prisms, m. 150-1°. VII with O_3 in EtOAc gave 1-tetralone. The Et_2O layer evapd. gave 1-cyanomethylene deriv. of Tetralin, m. 69-70° (aq. MeOH). Ozonolysis in EtOAc gave 1-tetralone. 2-Tetralone treated with Zn and I gave a product shown to be a mixt. of hydroxyester and unsatd. ester. The mixed esters (5 g.), 20 ml. H_2O, and 4 ml. 40% MeOH-KOH kept 24 hrs., warmed 20 min., and worked up as usual gave 2 substances. Crystn. gave prisms, m. 58-60°, subliming at 57-9°, m. 81-5°. Anal. data indicated that it was a mixt. of the hydroxyacid and its hydrate; acylurea, prisms, m. 154-5° (Me_2CO). The hydroxy acid (1 g.) warmed 3 hrs. with 1.5 g. Ac_2O and worked up in the usual manner gave 3,4-dihydro-2-naphthaleneacetic acid, m. 88-9°. The acid in Et_2O treated with Br gave 3a-bromo-2,3,3a,4,5,9b-hexahydronaphtho[1,2-b]furan-2-one, needles, m. 103-4° (ligroine). 1,1-Dimethyl-2-tetralone (21 g.) added to 9 g. Zn, 80 ml. C_6H_6, 80 ml. PhMe, and 20 g. I, the mixt. refluxed 1 hr., 20 g. I and 18 g. Zn added, refluxing continued 1 hr., the addn. of I and Zn repeated, after 2 hrs. further refluxing the mixt. cooled, decompd. by 3N HCl, the aq. layer extd. with C_6H_6, the combined org. layers washed, and distd. gave 12 g. Et 1,2,3,4-tetrahydro-2-hydroxy-1,1-dimethyl-2-naphthaleneacetate (VIII), b10 173-6°. VIII (2.5 g.), 10 ml. H_2O, and 2 ml. 40% MeOH-KOH kept 24 hrs., warmed 20 min. at 60°, dild., and acidified gave a ppt.; extn. with Et_2O followed by extn. with $NaHCO_3$ soln. and acidification gave the hydroxy acid-H_2O, m. 75-6° (capillary); acylurea m. 163-4°. The hydroxy ester (5 g.) heated 20 min. with 25 ml. HCO_2H and fractionated gave 3.5 g. yellow liquid, b10 170-5°, hydrolyzed by 40% MeOHKOH to the hydroxy acid, m. 101-2° (ligroine). Attempts to dehydrate the acid were unsuccessful. 1-Indanone (26.5 g.), 13 g. Zn, 150 ml. C_6H_6, and 33.4 g. I gave Et-3-indeneacetate (IX), b2 152-6°. IX (10 g.) refluxed 2 hrs. with 12 ml. 6N NaOH in 150 ml. MeOH, evapd., the soln. acidified, and the ppt. crystd. gave 6 g. 3-indeneacetic acid (X), m. 95-6° (ligroine); acylurea, prisms, m. 163-4°. X (3 g.) refluxed with 60 ml. dil. H_2SO_4 yielded 3-methylindene, b9 72-4°; picrate m. 77-9°; 1-(p-anisylidene) deriv. m. 111-12°. X (0.2 g.) and 0.25 g. p-anisaldehyde in 5 ml. alc. with 4 ml. alc.-KOH gave on acidification after 1 hr. the 1-(p-anisylidene) deriv., prisms, m. 178-80° (decompn.). X in Et_2O with Br gave the bromo lactone, prisms, m. 152-4° (Et_2O-ligroine). 2-Indanone (13.2 g.), 6.5 g. Zn, 16.7 g. I, and 150 ml. C_6H_6 was warmed, 0.5 g. iodine added, 2 addns. of 8 g. Zn and 20 g. I made after 1 and 2 hrs., the mixt. refluxed 2 hrs., the cooled soln. decompd. by 3N HCl, the aq. layer extd. with C_6H_6, dried, and distd. The residue with Et_2O yielded 1.2 g. solid, m. 216-17°. This was possibly the condensation product, 1,3-di(2-indanylidene)indan. Removal of the Et_2O gave 33% Et 2-hydroxy-2-indanacetate, b10 162-6°. The hydroxy ester (5 g.) warmed 0.5 hr. with 30 ml. HCO_2H gave 3.5 g. unsatd.

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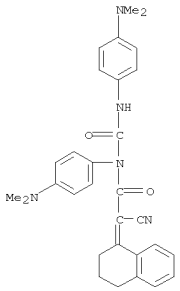
ester, b10 150-3°. The ester (3 g.) refluxed 2 hrs. with 4 ml. 6N NaOH and 40 ml. alc., evapd., and acidified gave 2-indeneacetic acid, prisms, m. 116-17° (ligroine); acylurea, prisms, m. 160-2°. The acid with dil. H_2SO_4 gave a solid, possibly the trimer of 2-indeneacetic acid, prisms, m. 228-30° (aq. alc.).

IT 103276-39-7P, Carbanilide, N-[cyano(3,4-dihydro-1(2H)-naphthylidene)acetyl]-4,4'-bis(dimethylamino)-
RL: PREP (Preparation)
(preparation of)

RN 103276-39-7 CAPLUS

CN Acetamide, 2-cyano-2-(3,4-dihydro-1(2H)-naphthalenylidene)-N-[4-(dimethylamino)phenyl]-N-[[[4-(dimethylamino)phenyl]amino]carbonyl]- (CA INDEX NAME)



L21 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1949:679 CAPLUS
DOCUMENT NUMBER: 43:679
ORIGINAL REFERENCE NO.: 43:168c-i,169a-b
TITLE: A new group of sweet substances
AUTHOR(S): Petersen, Siegfried; Muller, Erwin
SOURCE: Chemische Berichte (1948), 81, 31-8
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB In the course of investigations of high-mol. compds. from diisocyanates there was accidentally discovered a compound, 1-(2-carboxyethyl)-3-(p-nitrophenyl)urea (I), which, as the free acid and especially in the form of the alkali salts, is about 350 times sweeter than sucrose, and which, from physiol. studies to be reported later, is well tolerated by the animal organism. The Na salt has been designated Suosan.
I, gray-yellow crystals, m. 188°, is not particularly soluble in water (0.05 g. in 100 cc. at 20°, 0.75 g. at 100°), but the solubility of the Na salt is 6.2 and 60 g., resp., in 100 cc. of solution The salt, decompose 240°, has a deep yellow color which, however, is hardly noticeable at the concns. (0.1-0.2 g./l.) required for the sweetening of foods and beverages. NaOH solns. are orange, a color reaction which can be used for the detection of I. The salt can be comparatively readily salted out from its solns. and is quite stable to heat; long boiling in water splits off p-$O_2NC_6H_4NH_2$. I can be prepared in various ways. The simplest is the reaction of p-$O_2NC_6H_4NCO$ with β-alanine (or its nitrile, followed by hydrolysis), or the amino acid or nitrile can be converted into the corresponding isocyanate and condensed with p-$O_2NC_6H_4NH_2$. The nitrile corresponding to I can also be obtained from 1,1-bis(2-cyanoethyl)-3-(p-nitrophenyl)urea, m. 177-8°, with elimination of 1 mol. $CH_2{:}CHCN$, by heating 7 h. at 110° with alc. containing a small amount of NaOEt. The following compds. were prepared to determine the effect of various modifications of the I mol. on the taste (+++, very sweet; ++, distinctly sweet; ++), distinctly sweet with bitter aftertaste; +, faintly sweet; +), faintly sweet with bitter aftertaste; -, not sweet); m.ps. are given. p-$O_2NC_6H_4NHCONHR$: R = $CH_2CH_2CO_2H$ (I) 188°, +++; $CH_2CH_2CO_2Et$ 117°, -; $CH_2CH_2CONHNH_2$ 210-12°, -; CH_2CH_2CN 189-91°, -; CH_2CO_2H 201-3°, ++; $CHMeCO_2H$ 167°, -; $CHMeCH_2CO_2H$ 175-7°, ++); $CH_2CH_2CH_2CO_2H$ 166-7°, -; $CH_2(CH_2)_4CO_2H$ 163-4°, -; $CH_2CH_2SO_3H$ above 220°, -. p-$O_2NC_6H_4NHCONMeCH_2CO_2H$ 152°, -. p-$O_2NC_6H_4NHCON(CH_2CH_2CO_2H)_2$ 207°, -. RNHCONHCH2CH2CO2H: R = m-$O_2NC_6H_4$ 169-70°, +): o-$O_2NC_6H_4$ 167°, -; 2,4-Me(O2N)C6H3 190°, -; 2,4-Cl(O2N)C6H3 187°, -; p-$H_2NC_6H_4$ above 250°, -; p-$EtOC_6H_4$ 181-2°, -; 6,3-PrO(O2N)C6H3 207°, -; 6,3-MeO(O2N)C6H3 184-5°, -; 2,4-MeO(O2N)C6H3 192°, -. In the following, R = p-$O_2NC_6H_4$: RNHCOCH2CH2CO2H 196-7°, ++); RCONHCH2CH2CO2H 160-1°, +); RNHCSNHCH2CH2CO2H (II) 152-3°, +++; RNHCSNHCH2CO2H 158°, +; RNHCSNHCHMeCH2CO2H 185°, ++). The most interesting observation is that II, the S analog of I, is even sweeter than I; the Na salt is very soluble and cannot be salted out but its practical value is limited by the fact that physiol. it is less well tolerated than I. The following intermediate products in the preparation of

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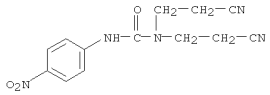
the above compds. are described: Et δ-(p-nitrophenyl)hydantoate, from p-$O_2NC_6H_4NH_2$ and $OCNCH_2CO_2Et$ refluxed 16 h. on the water bath, needle from MeOH, m. 166-7°. Substituted Ph isocyanates (m.p. of methylurethane in parentheses): 3-nitro-6-propoxy, not isolated in free form (methylurethane, m. 84-6°), from 6,3-PrO(O2N)C6H3NH2 and COCl2 in PHCl; 2-methyl-4-nitro, b2 168°, m. 75-8° (147-8°); 2-chloro-4-nitro, m. 62° (138-8.5°); 6-methoxy-3-nitro, m. 113° (134-5°); 2-methoxy-4-nitro, m. 115-16° (146-7°). 1-(p-Aminophenyl)-3-(2-cyanoethyl)-urea, from the nitro compd. in pyridine at 50° treated with dil. HCl and then slowly with Zn dust and heated 1 h. at 90°, m. 148-9°. β-(p-Nitrobenzamido)propionitrile, from $H_2NCH_2CH_2CN$ in acetone with p-$O_2NC_6H_4COCl$, m. 151-3°. 1-(2-Cyanoethyl)-3-(p-nitrophenyl)-2-thiourea, from p-$O_2NC_6H_4NCS$ in MeOH and $H_2NCH_2CH_2CN$, m. 154-6° (from glacial AcOH), also obtained from $NCCH_2CH_2NCS$ and p-$O_2NC_6H_4NH_2$.

IT 23993-79-5P, Urea, 1,1-bis(2-cyanoethyl)-3-(p-nitrophenyl)-
74390-17-3P, Urea, 1-(2-cyanoethyl)-3-(p-nitrophenyl)-
688341-37-9P, Urea, 1-(p-aminophenyl)-3-(2-cyanoethyl)-
RL: PREP (Preparation)
(preparation of)

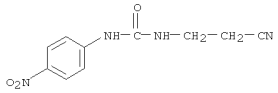
RN 23993-79-5 CAPLUS

CN Urea, 1,1-bis(2-cyanoethyl)-3-(p-nitrophenyl)- (8CI) (CA INDEX NAME)



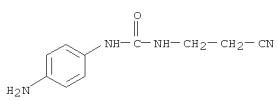
RN 74390-17-3 CAPLUS

CN Urea, N-(2-cyanoethyl)-N'-(4-nitrophenyl)- (CA INDEX NAME)



RN 688341-37-9 CAPLUS

CN Urea, N-(4-aminophenyl)-N'-(2-cyanoethyl)- (CA INDEX NAME)



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ACCESSION NUMBER: 1939:59656 CAPLUS
DOCUMENT NUMBER: 33:59656
ORIGINAL REFERENCE NO.: 33:8567b-i,8568a-i,8569a-c
TITLE: Characterization of carboxylic acids as ureides by means of carbodiimides. IV. A test for α,β-unsaturated acids
AUTHOR(S): Zetzsche, Fritz; Rottger, Gerhard
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1939), 72B, 1599-612
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C. A. 33, 3771.4. The N-acyl-N,N'-bis(4-dimethylaminophenyl) ureas, RCON(C6H4NMe2)CONHC6H4NMe2, easily obtained from carboxylic acids and the "basic" carbodiimide C(:NC6H4NMe2)2 (I), are colored when R : R'CH:CH or R'C.tplbond.C, whereas those having an unsatd. union in another than the α,β-position are colorless. On the other hand, the p-tolylureas are colorless unless the acid itself is colored, in which case the ureide is not more deeply colored. 2-Hentriacontenoic acid shows that the color effect, which decreases in intensity from acrylic to the C31-acid, persists unmistakably far up the n-alkylacrylic acid series, and the limit of detectability should extend far beyond the C31-acid. The color also appears in the α,β-acetylenecarboxylic acids (propiolic, tetrolic). Conjugated Δ2,4-acids (sorbic, piperic), as also cinnamic and furfuracrylic acids, show, as compared with β-alkyleneacrylic acids with non-conjugated double bond (geranic acid) and β-alkylacrylic acids, a deepening of the color (to red-orange in sorbic and cinnamic, and to red in piperic acid). Inner complex salt formation has the same effect (the fumaric monoureide is red). The basic ureides of α-alkylated or α-arylated acrylic acids of the type RCH:CR'CO2H and CH2:CR'CO2H show such a slight deepening of color, as compared with those of the n-acrylic acids, that they are colorless or only faintly yellow. This phenomenon is designated the "α-effect," for the corresponding β,β-dialkylation appears, as shown by comparison with geranic and cyclohexylideneacetic acids, to exert no such pronounced effect, although there seems to be some weakening of the color. The ureide of Δ1,4-dihydrobenzoic acid, which may be considered as an α-alkylacrylic acid, is colorless. Aromatic carboxylic acids give in part colored, in part colorless, basic ureides but it is not surprising that they should show greater diversity than acids of the acrylic acid series. Nevertheless, introduction of the basic urea residue in benzoic, anisic and piperonylic acids has such a color-deepening effect that the ureides have a yellow (even if but faint) color. α- and β-Naphthoic acids, and also iso- and terephthalic acids, can be readily distinguished from each other by the color of their ureides. In the heterocyclic series with an aromatic state of saturation, β-pyridinecarboxylic acid, with its pale yellow ureide, falls in with BzOH, while the α-acid gives a colorless ureide. The color deepening is especially marked with furan- and thiophene-α-carboxylic acids. Hence, direct union of an aromatic system with the carboxyl group in the basic ureides has approx. the same effect as an α-ethylene group. Union through aliphatic groups (Ph2CHCO2H, 1-pyrenylbutyric acid, PhCH2CH2CO2H) or with hydrogenated ring members

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(9,10-dihydroanthracene-9-carboxylic acid) does not, any more than an accumulation of double bonds not in the α-position in olefin carboxylic acids (linoleic, linolenic), suffice to increase any possible color deepening which may be produced enough to make the color visible. Z. and R. do not as yet offer any interpretation of the cause of the color of their compds., for they have encountered similar phenomena in another group of carboxylic acids, and they consider it necessary to include other basic carbodiimides and carboxylic acids in their study. Moreover, the occurrence of 2 differently colored forms of the ureide found with sorbic acid is apparently not at all an isolated case. Since the color and color change in the basic ureides not only must be conditioned by a conjunction of α,β-unsatd. carboxylic residues and the basic ureide group but may also be brought about by the interplay of other factors, it is not surprising that the introduction of the basic urea residue with its 2 strong auxochromic residues NMe2 into powerful chromogens should likewise produce a deepening of the color; thus, the basic ureide of the yellow 1-β-pyrenoylpropionic acid is green. These facts do not affect the applicability of the new method, by which it is now possible to characterize carboxylic acids in general as their ureides and to detect certain structural peculiarities (detection of the proximity of the CO2H groups in polybasic acids by the formation of anhydrides, or of α,β-unsatd. unions by the formation of colored ureides). The yields of the ureides described in this paper were generally about 90%. The mother liquors were always worked up by evapg. at room temp. in vacuo and recrystg. the residue. The detection of even faint colors is greatly facilitated by the fact that most of the ureides crystallize not only excellently but in compact thick crystals. In detg. the m. ps. it should be remembered that the monoacylureas readily decomp. into an isocyanate and acid arylide, frequently in the vicinity of the m. p., and as the acyl arylides generally melt higher than the ureides and the isocyanates are in part liq. at the m. p. and in part very poor solvents for the arylides, the melt often resolidifies and melts again at a higher temp., or the ureide decomp. on slow heating without melting until approx. the m. p. of the arylide is reached. Ureides from I with the following acids: acrylic, strongly yellow, sinters 141°, m. 144.5°; α-crotonic, yellow, m. 150° (cor.); 2-hexenoic, yellow, sinters 137°, m. 139°; 2-octadecenoic, light yellow, sinters 113°, m. 115°; 2-hentriacontenoic, light yellow, m. 103-4°; cyclohexylideneacetic, light yellow, sinters 149°, m. 151°; sorbic, orange clumps and short yellow crystals (both forms sep. from acetone in yellow squares; the orange form can be obtained only directly by prepn. of the ureide in ether and only by rapid crystn. from very concd. soln.; it changes at about 100° into the yellow form, which sinters 145°, m. 147°); geranic, light yellow, m. 126-7°; fumaric, red, sinters 166°, m. 168°, changes on short boiling (45-60 s.) in a little sec-octyl alc. into yellow needles, m. around 300°; cinnamic, orange, sinters 153°, m. 155.5°; furfuracrylic, brown-orange, m. 153-4° (cor.); piperic, bright red, sinters 153°, m. 154° to an orange-yellow liq. resolidifying at 155° and m. again about 185° to a red liq.; acetylenecarboxylic, deep yellow, sinters 129°, m. 132°; tetrolic, yellow, sinters 139°, m.

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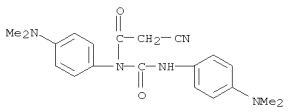
141-2°; phenylpropiolic, yellow, sinters 149°, m. 151°; 3-hexenoic, colorless, sinters 144°, m. 146° (cor.); benzalpropionic, yellowish white, m. 150-2°; 3-hexene-1,6-dioic, colorless, m. 210°; allylacetic, colorless, m. 148-9° (cot.); cis-15-tetracosenoic, white, m. 96-7°; trans-isomer, white, m. 110-11.5°; α-cyclogeranic, pure white, m. 142-3°; chaulmoogric, colorless, sinters 115°, m. 116.5°; methacrylic, white, sinters 140°, m. 143.5°, mol. wt. in benzene 346; tiglic, colorless, sinters 135°, m. 137°; atropic, yellowish white, m. 134-5°; α-methylcinnamic, light yellow, sinters 135°, m. 139°; α-phenylcinnamic, light yellow, sinters 151°, m. 152.5°; Δ1,4-dihydrobenzoic, yellowish white, m. 148-9° (decompn.); benzoic, faintly yellow, m. 198-218°, depending on the rate of heating, at once when placed in a bath preheated to 160°; p-toluic, very faintly yellow, m. 147-8°; anisic, exceedingly faintly yellow, m. 151-3°; piperonylic, pale yellow, m. 135-6°; hydrocinnamic, colorless, m. 155-6°; terephthalic, deep yellow, becomes discolored about 180°, darkens 200°, sinters about 240°, decomp. on further heating without melting up to 320° (when it is boiled a few min. in sec-octyl alc. the color lightens and there sep. light yellow needles of terephthalylbis(4-dimethylaminophenylimide), decomp. without melting when heated up to 340°); isophthalic, pale yellow, bakes to a moist cake at 162°, dry at about 190°, m. 205-15° (decompn.) (in a bath preheated to 190° it melts, resolidifies at once and m. 215-25° (decompn.); boiling 7 min. in secoctyl alc. converts it into the bisimide); α-naphthoic, pale yellow, m. 162° (decompn.); β-naphthoic, yellow, m. 185-90° (170° in a preheated bath); anthracene-9-carboxylic, deep yellow, sinters 177°, m. 180°; 9,10-dihydro deriv., colorless, m. 119-21°; diphenylacetic, white. m. 154-5°, resolidifies a few degrees higher and again m. 180°; 2',4'-dimethoxybenzophenone-2-carboxylic, yellow, m. 154-5.5°; β-1-pyrenoylpropionic, green; γ-1-pyrenylbutyric, yellowish white, m. 153-5°; furan-α-carboxylic, yellow, sinters 136°, m. 141°; thiophene-α-carboxylic, yellow-orange, m. 136.5-7°; nicotinic, pale yellow, sinters 128°, m. clear 150°; pyridine-α-carboxylic, colorless, sinters 150°, m. 154°; cyanoacetic, pure white, sinters 255°, m. 262°. Contrary to almost all the other ureides, that of p-phthalic acid is difficultly sol. in CHCl3, and can be used for the sepn. of the p- from the m-acid; by this means 2 com. samples of isophthalic acid were found to contain 4.4-4.5% p-acid.

IT 855180-92-6P, Carbanilide, N-cyanoacetyl-4,4'-bis(dimethylamino)-
RL: PREP (Preparation)
(preparation of)

RN 855180-92-6 CAPLUS

CN Acetamide, 2-cyano-N-[4-(dimethylamino)phenyl]-N-[[[4-(dimethylamino)phenyl]amino]carbonyl]- (CA INDEX NAME)

L21 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-14.40	-19.20

STN INTERNATIONAL LOGOFF AT 08:15:04 ON 20 OCT 2008